LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008729.D
Acq On : 07 Jan 2022 16:49
Operator : CG/JU
Sample : N1049-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
7211979

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008729.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.023	3	6	10	rVB2	449524	528602	2.90%	0.305%
2	3.070	10	14	22	rVB	1778154	2320464	12.73%	1.337%
3	4.064	179	183	188	rBV	181941	243638	1.34%	0.140%
4	5.193	370	375	385	rVB	131674	200545	1.10%	0.116%
5	5.452	412	419	436	rBV	5548926	8572716	47.03%	4.939%
6	7.046	681	690	706	rBV	5823992	9183306	50.38%	5.290%
7	7.181	708	713	728	rVB3	59786	190006	1.04%	0.109%
8	7.869	820	830	838	rBV	1425218	2335230	12.81%	1.345%
9	8.534	936	943	953	rVB4	90519	218582	1.20%	0.126%
10	9.028	1020	1027	1039	rVB	3714474	6273382	34.42%	3.614%
11	10.452	1260	1269	1278	rBV	452174	802169	4.40%	0.462%
12	10.669	1297	1306	1314	rBV	1518227	2608885	14.31%	1.503%
13	12.857	1669	1678	1681	rBV3	126657	296849	1.63%	0.171%
14	12.946	1687	1693	1703	rVB2	181861	325467	1.79%	0.187%
15	13.040	1703	1709	1714	rBV3	193264	444952	2.44%	0.256%
16	13.134	1714	1725	1731	rBV	7836661	12471653	68.42%	7.185%
17	13.263	1742	1747	1751	rBV	222600	397596	2.18%	0.229%
18	13.304	1751	1754	1759	rVB	158464	236821	1.30%	0.136%
19	13.416	1768	1773	1776	rBV6	127371	232118	1.27%	0.134%
20	13.575	1794	1800	1806	rVB	598542	1050648	5.76%	0.605%
21	13.663	1807	1815	1819	rBV2	225816	430002	2.36%	0.248%
22	13.787	1830	1836	1840	rBV3	307704	570125	3.13%	0.328%
23	14.163	1896	1900	1906	rBV4	120413	228446	1.25%	0.132%
24	14.357	1928	1933	1940	rBV4	197560	380541	2.09%	0.219%
25	14.469	1948	1952	1954	rBV	502941	680424	3.73%	0.392%
26	14.504	1954	1958	1963	rVV	2415214	3650058	20.02%	2.103%
27	14.551	1963	1966	1971	rVB	226153	293165	1.61%	0.169%
28	14.693	1986	1990	1994	rVB2	231584	311964	1.71%	0.180%
29	14.740	1995	1998	2002	rBV3	113108	187040	1.03%	0.108%
30	14.904	2023	2026	2029	rBV2	216220	309461	1.70%	0.178%
31	15.457	2117	2120	2127	rVB	530319	678304	3.72%	0.391%
32	15.998	2206	2212	2219	rBV	6960683	10246397	56.21%	5.903%
33	16.663	2321	2325	2332	rVB	1875084	2648281	14.53%	1.526%
34	16.734	2333	2337	2341	rBV	550258	779243	4.27%	0.449%
35	17.257	2422	2426	2435	rVB	2940044	4592742	25.20%	2.646%
36	17.351	2438	2442	2446	rVV	1173116	1565871	8.59%	0.902%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008729.D
Acq On : 07 Jan 2022 16:49
Operator : CG/JU
Sample : N1049-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 7211979

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	18.063	2559	2563	2572	rVB	933624	1291492	7.09%	0.744%
38	18.163	2575	2580	2585	rVB	2875147	4126401	22.64%	2.377%
39	18.986	2716	2720	2726	rVB	3068683	3990643	21.89%	2.299%
40	19.051	2727	2731	2739	rVB	927330	1570308	8.61%	0.905%
41	19.392	2785	2789	2798	rVB	2970735	4180849	22.94%	2.408%
42	19.510	2806	2809	2814	rBV	1763611	2219415	12.18%	1.279%
43	19.575	2818	2820	2822	rVV	517527	517620	2.84%	0.298%
44	19.604	2823	2825	2829	rVB2	668266	683173	3.75%	0.394%
45	19.733	2844	2847	2854	rVB	763744	1044776	5.73%	0.602%
46	19.822	2857	2862	2867	rVB	14457989	18228481	100.00%	10.501%
47	20.033	2894	2898	2902	rVB	1654800	1944348	10.67%	1.120%
48	20.286	2937	2941	2946	rVB3	879599	1393350	7.64%	0.803%
49	20.504	2975	2978	2984	rVB	1507226	1926898	10.57%	1.110%
50	20.704	3008	3012	3015	rVB	923439	1066826	5.85%	0.615%
51	20.751	3016	3020	3023	rVV	3065178	3615373	19.83%	2.083%
52	20.810	3027	3030	3034	rVB	1117654	1207969	6.63%	0.696%
53	21.063	3070	3073	3079	rVB3	1038724	1372753	7.53%	0.791%
54	21.157	3085	3089	3091	rBV	920958	1348419	7.40%	0.777%
55	21.186	3091	3094	3100	rVB	2825525	3320660	18.22%	1.913%
56	21.245	3101	3104	3112	rVB2	1526154	2144811	11.77%	1.236%
57	21.345	3117	3121	3132	rVB	4448497	7478790	41.03%	4.308%
58	21.469	3138	3142	3147	rBV	1782250	2560353	14.05%	1.475%
59	21.622	3164	3168	3174	rVB	1628541	2178841	11.95%	1.255%
60	21.969	3223	3227	3234	rVB2	1182026	2596877	14.25%	1.496%
61	22.092	3245	3248	3251	rVB	822661	960454	5.27%	0.553%
62	22.345	3287	3291	3298	rVB	2606611	3962528	21.74%	2.283%
63	22.422	3301	3304	3309	rVB	898585	1243863	6.82%	0.717%
64	22.886	3378	3383	3392	rBV2	2303182	4536516	24.89%	2.613%
65	23.469	3478	3482	3490	rVB	1103430	2058782	11.29%	1.186%
66	23.769	3528	3533	3542	rVB2	2665676	5611334	30.78%	3.233%
67	24.533	3656	3663	3672	rVB4	1813504	4955208	27.18%	2.855%
68	25.398	3806	3810	3823	rVB	787454	1764216	9.68%	1.016%

Sum of corrected areas: 173588020

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008729.D
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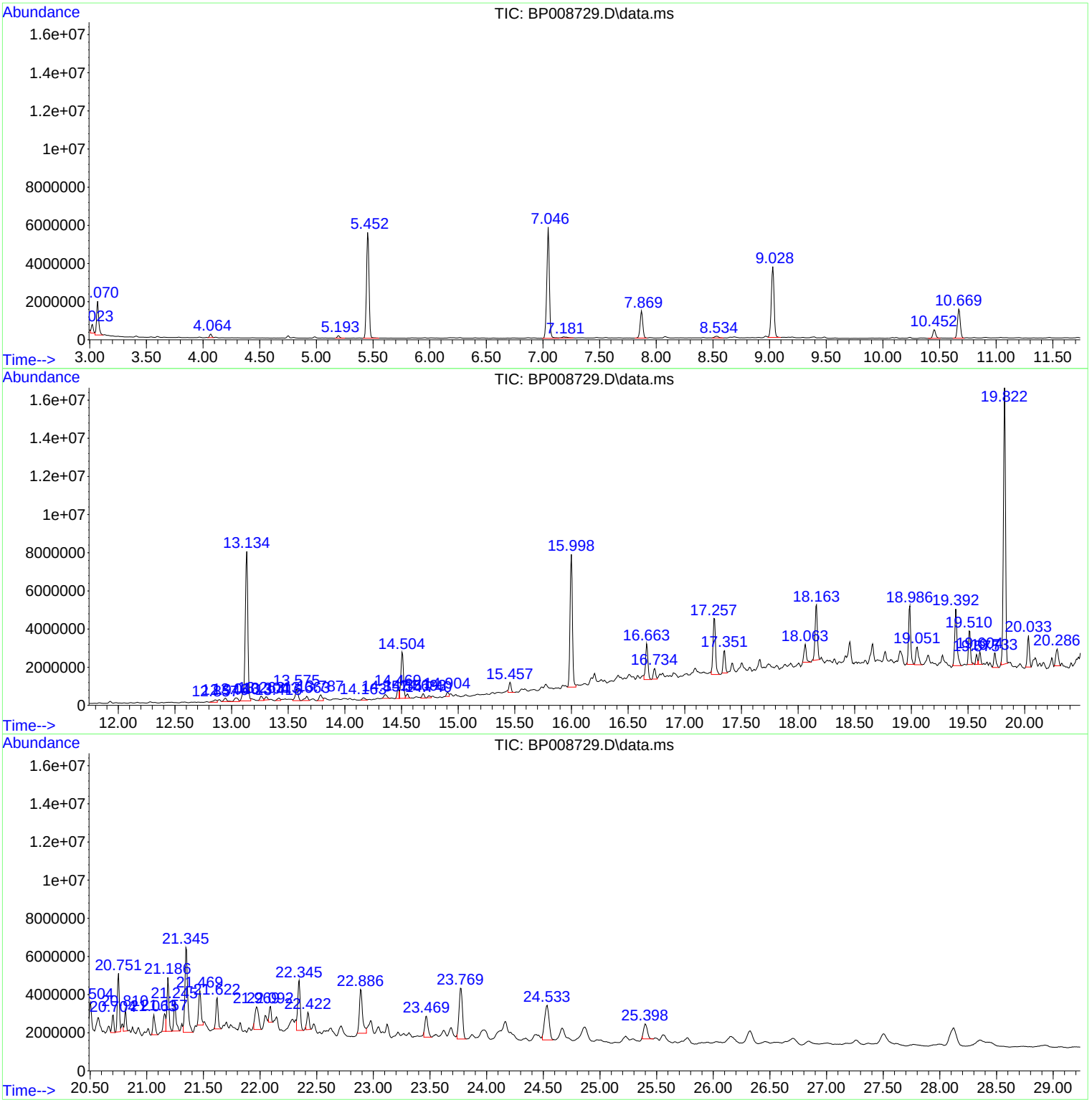
Sample : N1049-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
7211979

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008729.D
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Operator : CG/JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

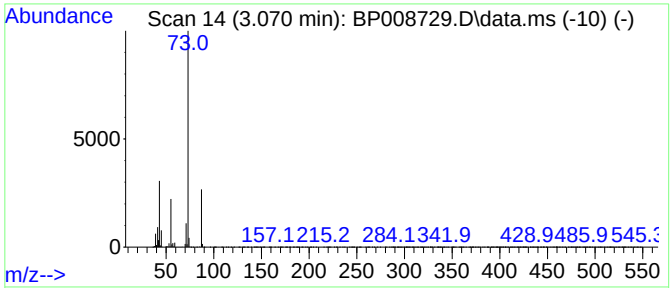
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

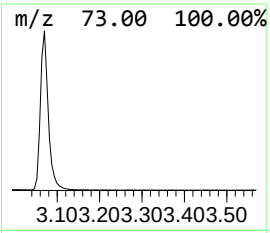
****

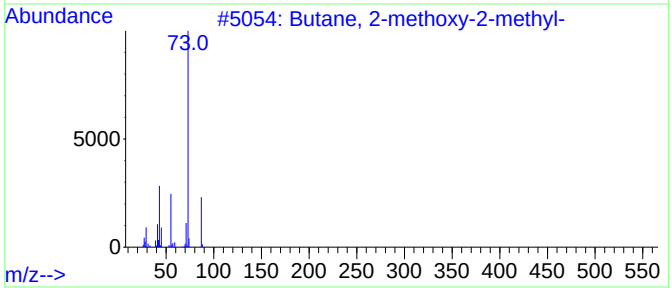
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

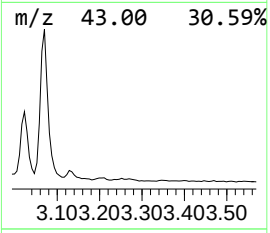
R.T.	EstConc	Area	Relative to ISTD	R.T.
3.070	19.87 ng	2320460	1,4-Dichlorobenzene-d4	7.869

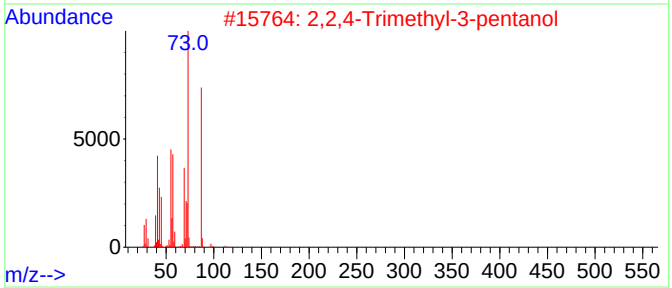
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9

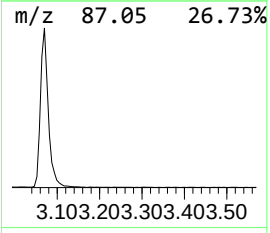


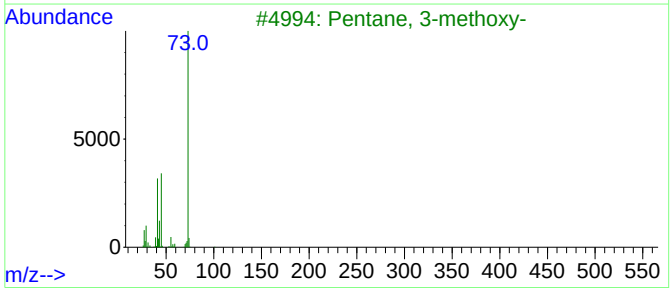


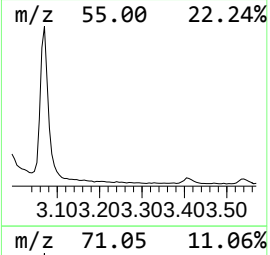


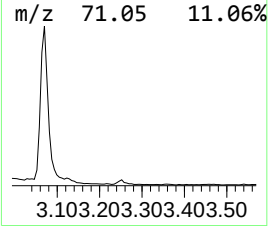












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008729.D
Acq On : 07 Jan 2022 16:49
Operator : CG/JU
Sample : N1049-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
7211979

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

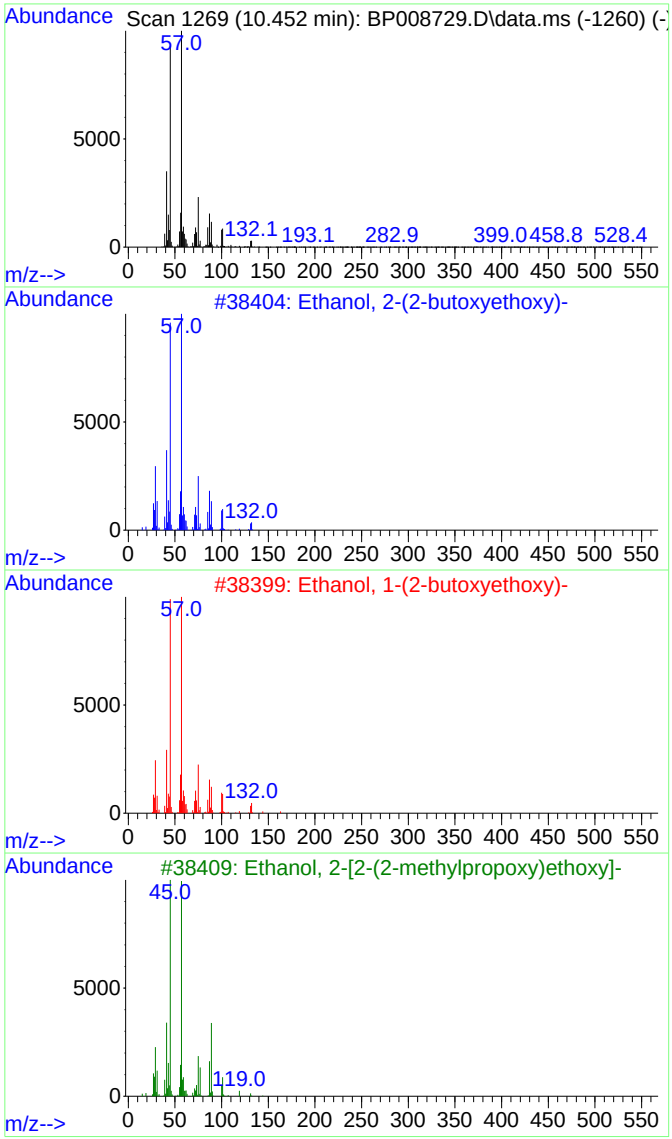
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

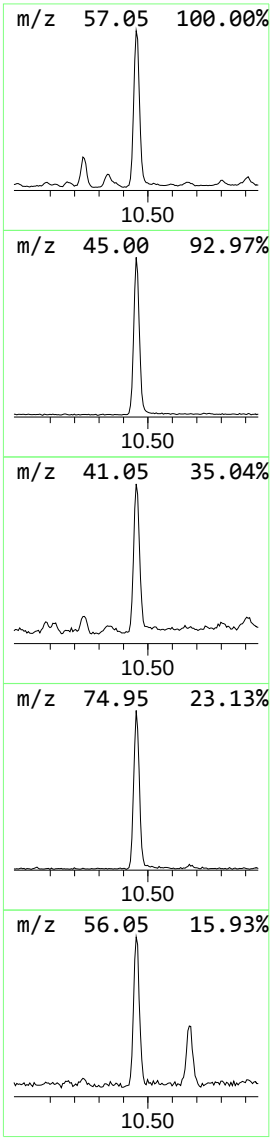
****

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.452	6.15 ng	802169	Naphthalene-d8	10.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	91
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	72
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
5	Hexane, 1-(methoxymethoxy)-	146	C8H18O2	066675-06-7	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008729.D
Acq On : 07 Jan 2022 16:49
Operator : CG/JU
Sample : N1049-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
7211979

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

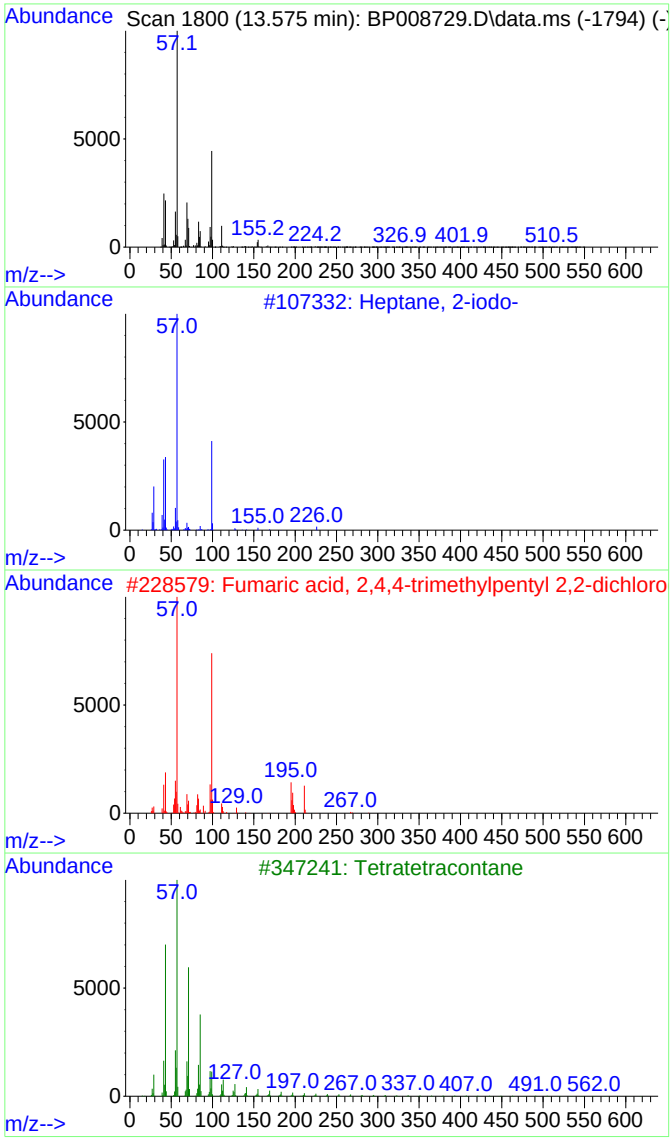
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

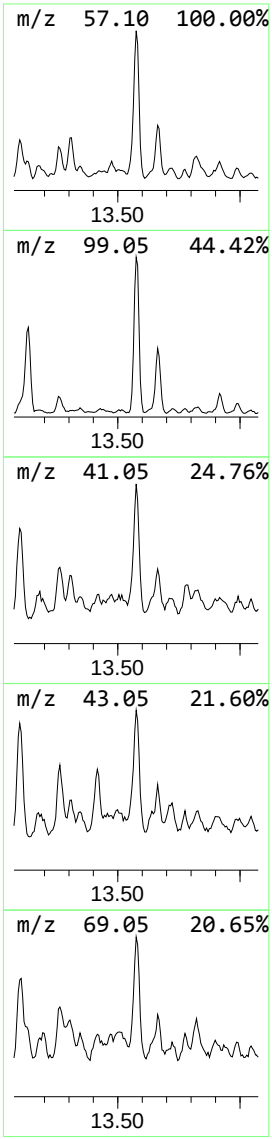
****

Peak Number 3 unknown13.575 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.575	5.76 ng	1050650	Acenaphthene-d10	14.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 2-iodo-	226	C7H15I	018589-29-2	43
2	Fumaric acid, 2,4,4-trimethylpen...	324	C14H22Cl2O4	1000405-60-4	40
3	Tetratetracontane	619	C44H90	007098-22-8	38
4	2-Azido-2,4,4,6,6,8,8-heptamethy...	267	C16H33N3	1000293-29-1	37
5	Diethylmalonic acid, monochlorid...	290	C15H27ClO3	1010369-49-2	36





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008729.D
Acq On : 07 Jan 2022 16:49
Operator : CG/JU
Sample : N1049-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
7211979

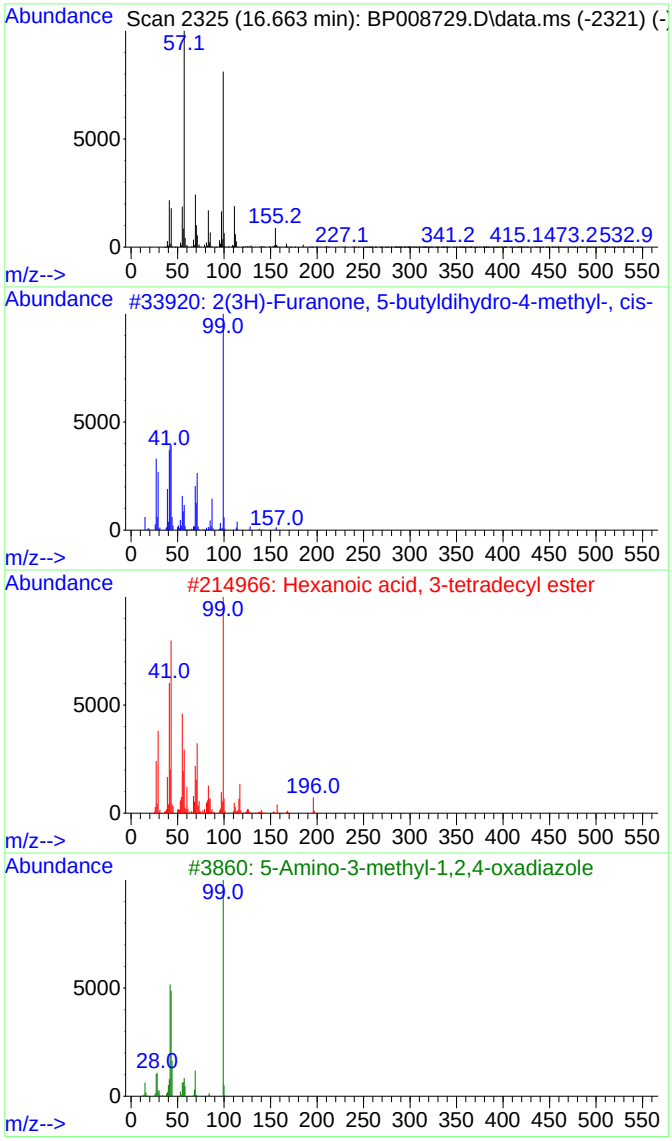
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

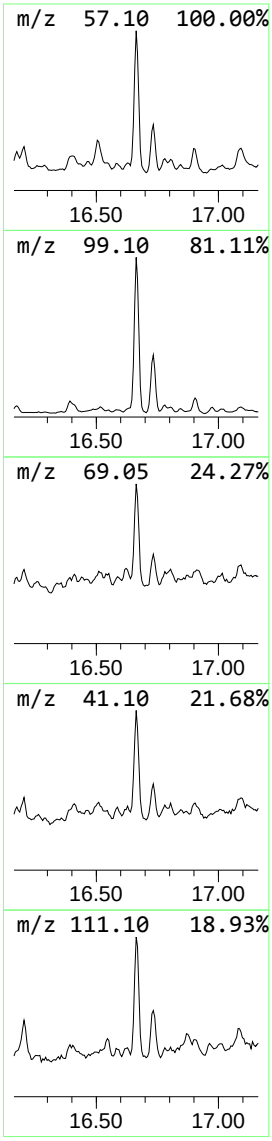
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2(3H)-Furanone, 5-butyldihy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.663	11.53 ng	2648280	Phenanthrene-d10	17.257

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Furanone, 5-butyldihydro-4...	156	C9H16O2	055013-32-6	53
2	Hexanoic acid, 3-tetradecyl ester	312	C20H40O2	1010279-29-7	53
3	5-Amino-3-methyl-1,2,4-oxadiazole	99	C3H5N3O	003663-39-6	50
4	Phosphonofluoridic acid, methyl-...	224	C10H22FO2P	211192-74-4	47
5	Malonic acid, di(2,4-dimethylpen...	300	C17H32O4	1000349-02-5	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008729.D
Acq On : 07 Jan 2022 16:49
Operator : CG/JU
Sample : N1049-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
7211979

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

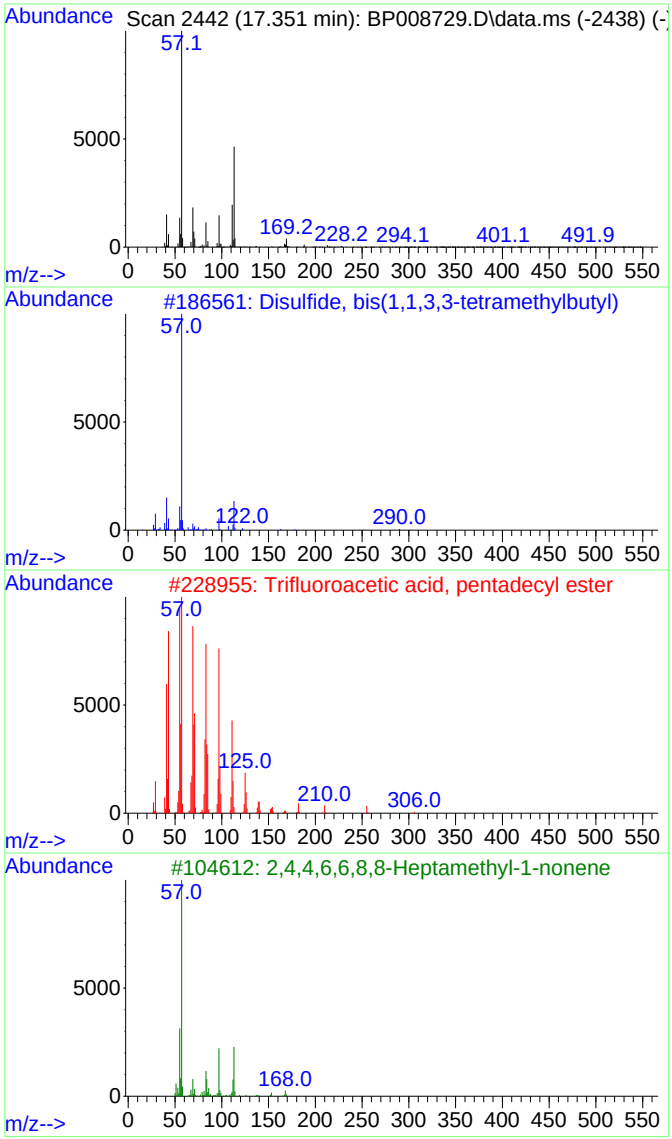
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

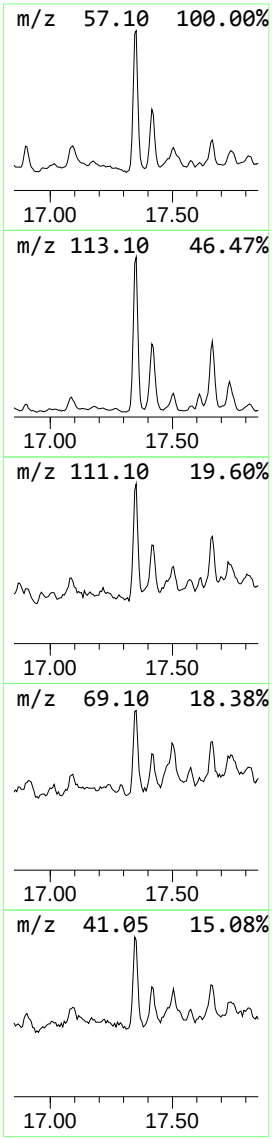
****

Peak Number 5 unknown17.351 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.351	6.82 ng	1565870	Phenanthrene-d10	17.257

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, bis(1,1,3,3-tetrameth...	290	C16H34S2	029956-99-8	38
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	27
3	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	23
4	5-Nonanone, 2,2,8,8-tetramethyl-	198	C13H26O	005709-95-5	17
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008729.D
Acq On : 07 Jan 2022 16:49
Operator : CG/JU
Sample : N1049-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

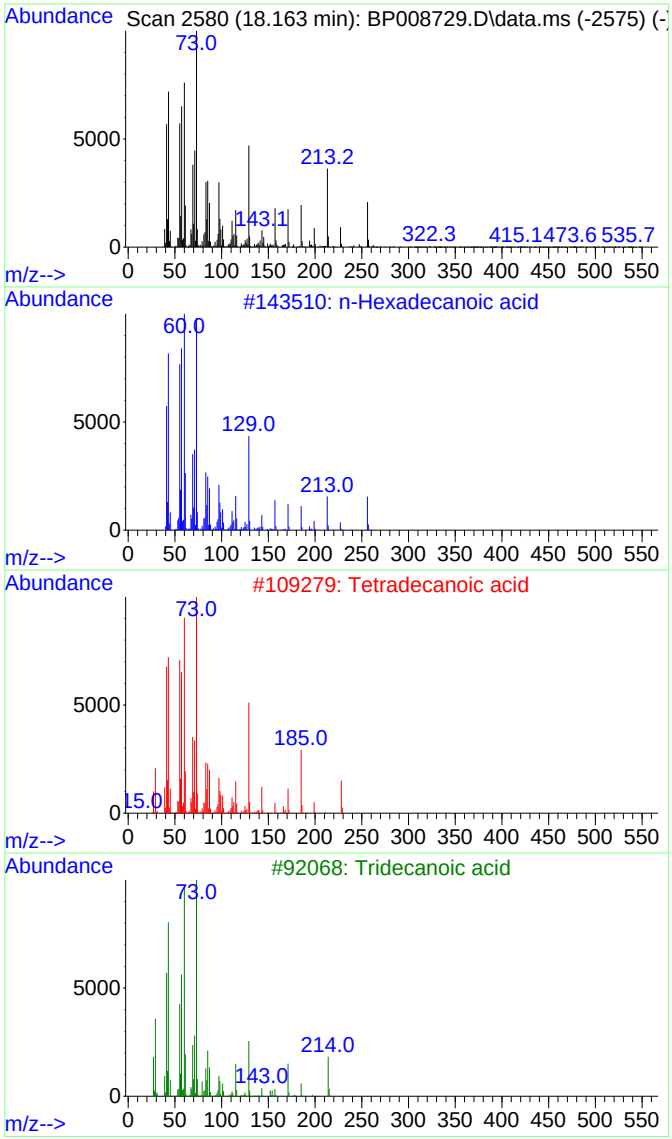
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

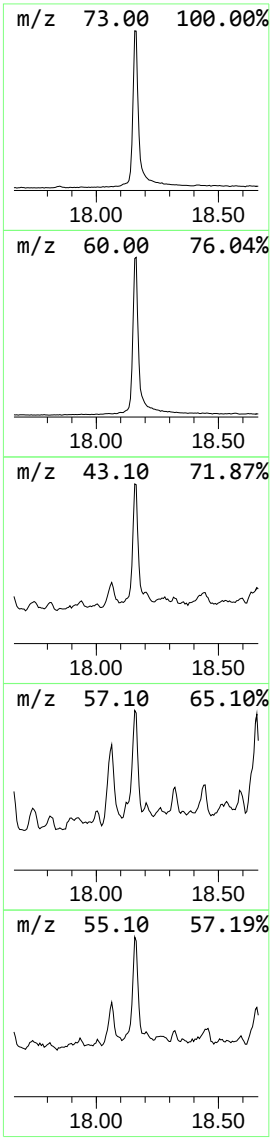
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.163	17.97 ng	4126400	Phenanthrene-d10	17.257

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	Octadecanoic acid	284	C18H36O2	000057-11-4	72
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	64





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Acq On : 07 Jan 2022 16:49
Operator : CG/JU
Sample : N1049-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
7211979

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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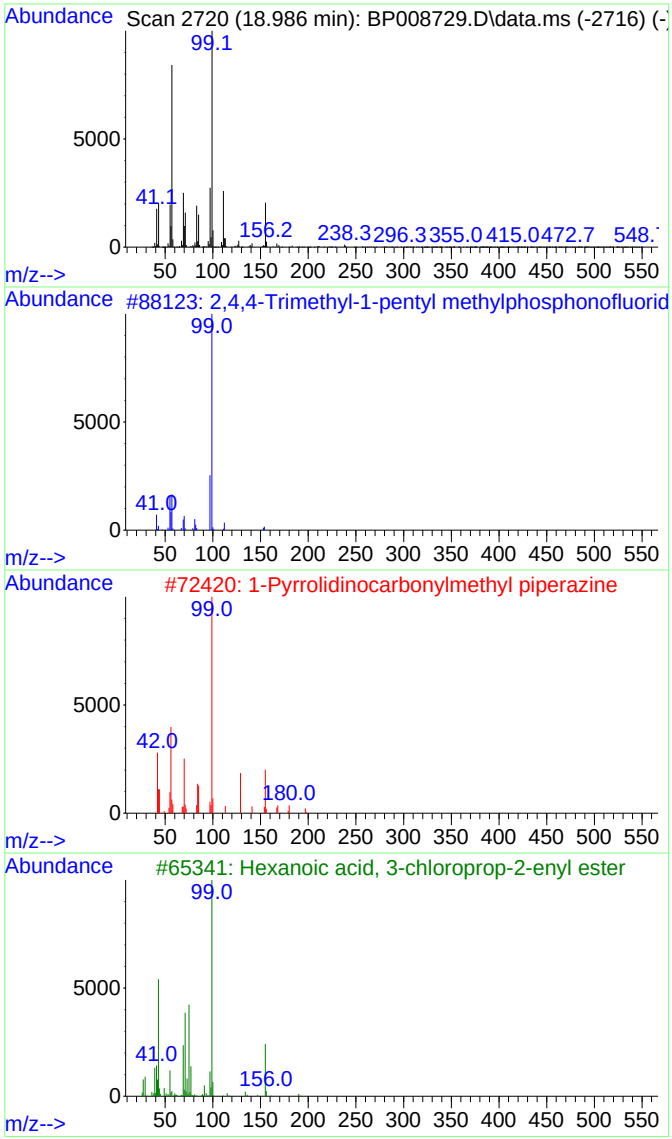
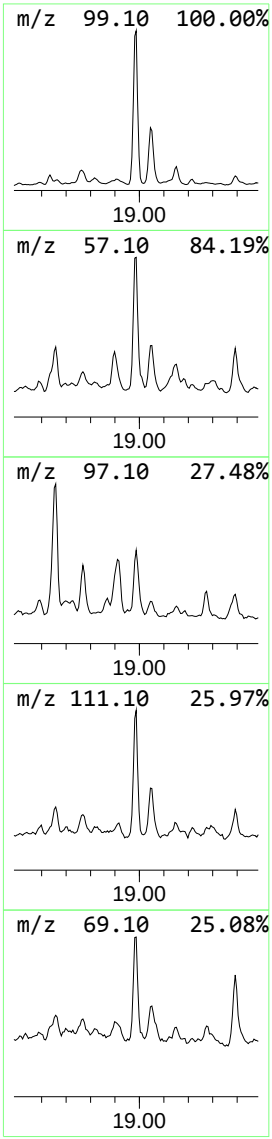
Peak Number 7 unknown18.986 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.986	17.38 ng	3990640	Phenanthrene-d10	17.257

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4-Trimethyl-1-pentyl methylp...	210	C9H20FO2P	333416-06-1	43
2	1-Pyrrolidinocarbonylmethyl pipe...	197	C10H19N3O	039890-45-4	43
3	Hexanoic acid, 3-chloroprop-2-en...	190	C9H15ClO2	1000299-36-1	43
4	4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	38
5	N-Phenyl-N'-(2-piperazin-1-yl-et...	276	C14H20N4O2	332404-00-9	35





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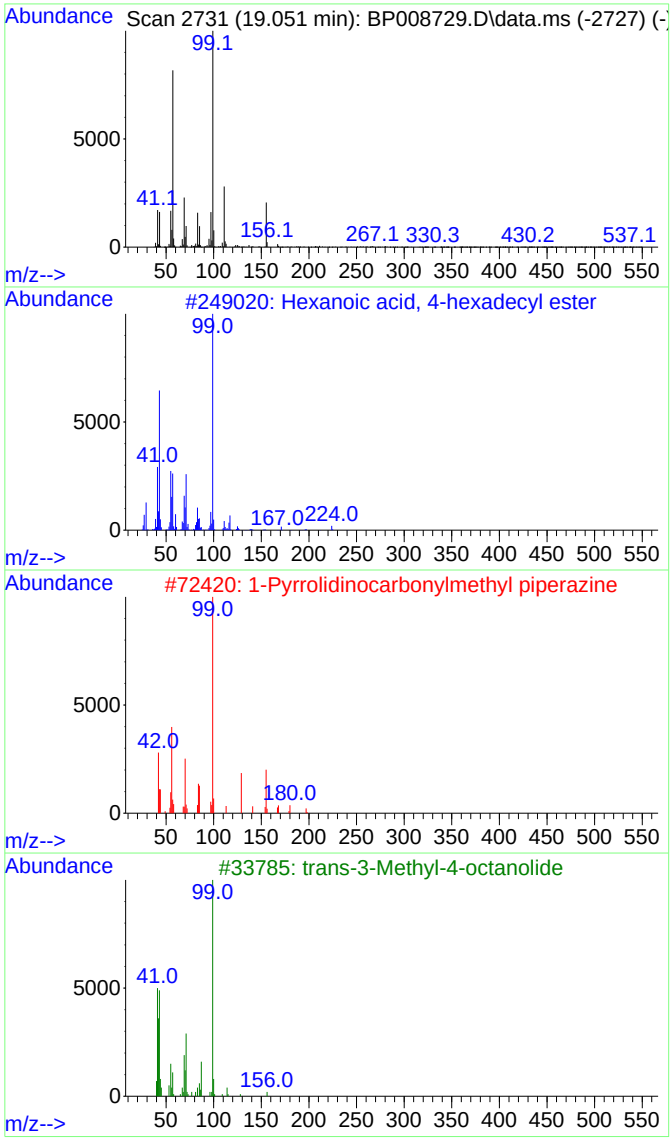
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

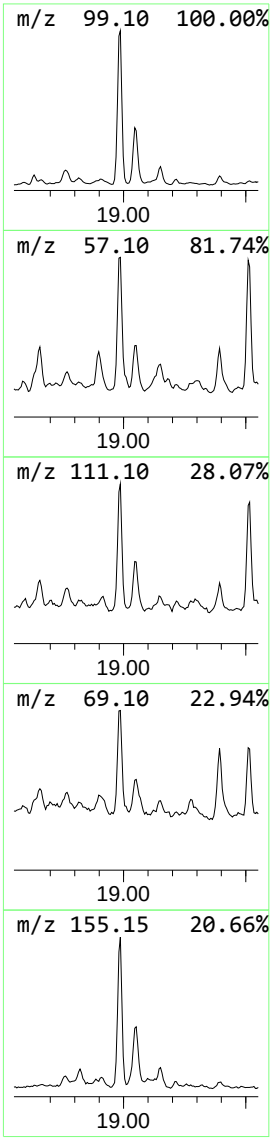
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Hexanoic acid, 4-hexadecyl ... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.051	6.84 ng	1570310	Phenanthrene-d10	17.257

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 4-hexadecyl ester	340	C22H44O2	1000282-83-8	50
2	1-Pyrrolidinocarbonylmethyl pipe...	197	C10H19N3O	039890-45-4	47
3	trans-3-Methyl-4-octanolide	156	C9H16O2	039638-67-0	47
4	4,8,12,16-Tetramethylheptadecan-...	324	C21H40O2	096168-15-9	42
5	Hexanoic acid, 3-chloroprop-2-en...	190	C9H15ClO2	1000299-36-1	40





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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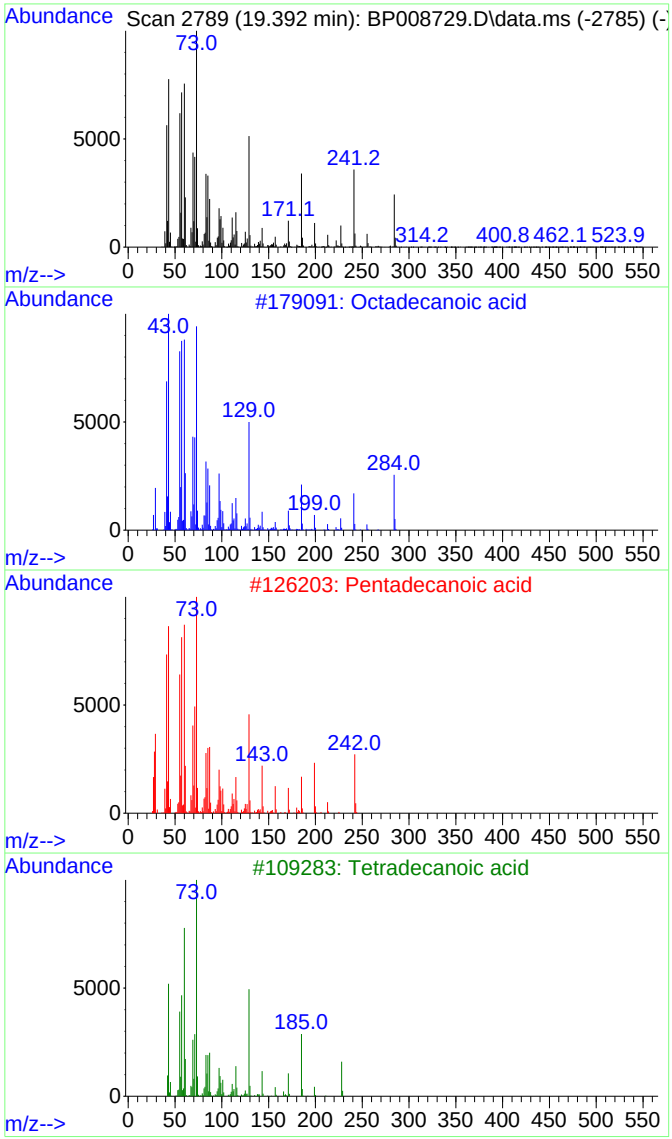
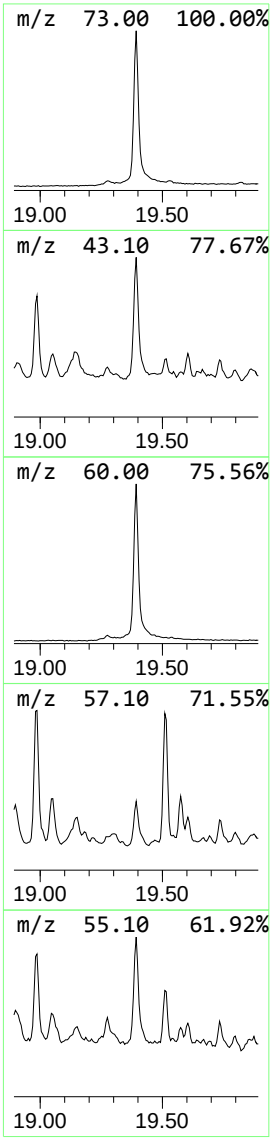
Peak Number 9 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.392	11.18 ng	4180850	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	62





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Misc :
ALS Vial : 8 Sample Multiplier: 1

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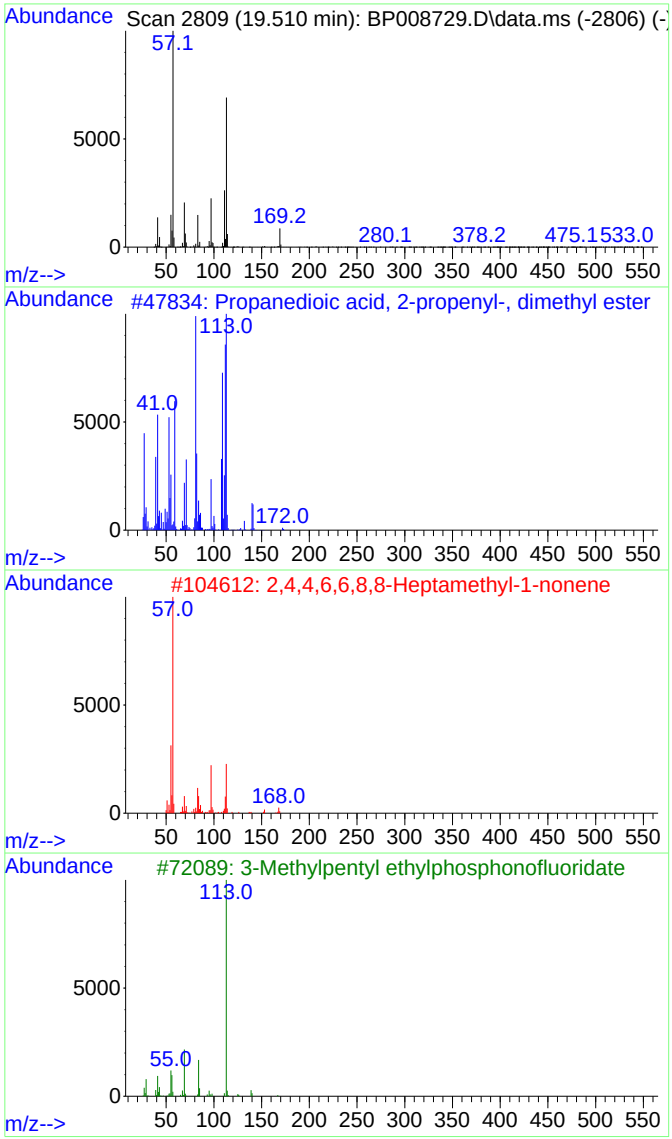
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

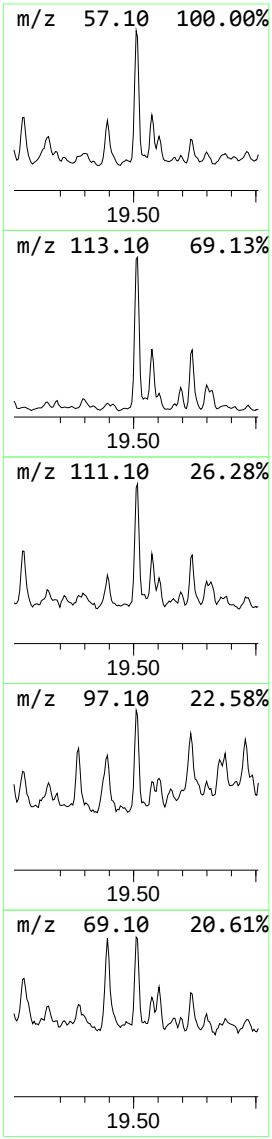
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Propanedioic acid, 2-propen... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.510	5.94 ng	2219420	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanedioic acid, 2-propenyl-, ...	172	C8H12O4	040637-56-7	53
2	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	28
3	3-Methylpentyl ethylphosphonoflu...	196	C8H18FO2P	1000298-39-1	22
4	2-Ethylhexyl ethylphosphonofluor...	224	C10H22FO2P	1000298-44-7	17
5	Borinic acid, diethyl-, (2-ethyl...	198	C9H20B2O3	058163-56-7	17





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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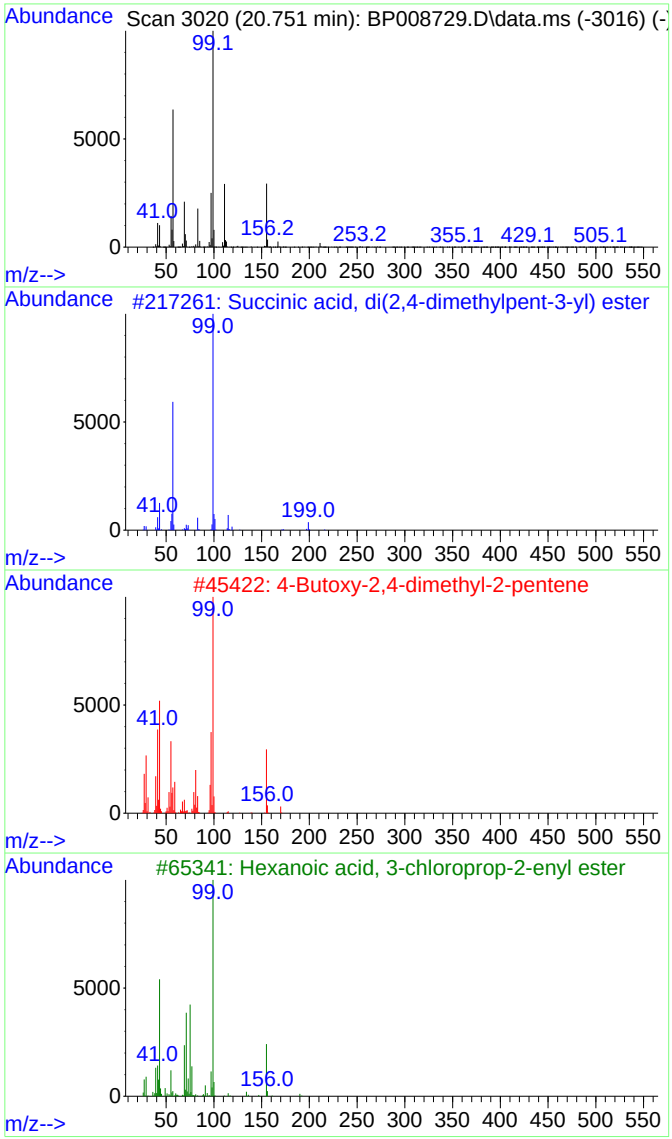
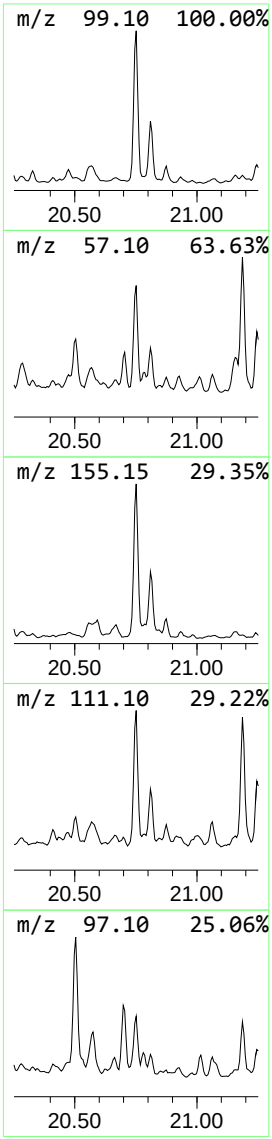
Peak Number 11 unknown20.751 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.751	9.67 ng	3615370	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Succinic acid, di(2,4-dimethylpe...	314	C18H34O4	1000349-36-7	47
2	4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	45
3	Hexanoic acid, 3-chloroprop-2-en...	190	C9H15ClO2	1000299-36-1	42
4	Tributyl phosphate	266	C12H27O4P	000126-73-8	40
5	2,4,4-Trimethyl-1-pentyl methylp...	210	C9H20FO2P	333416-06-1	38





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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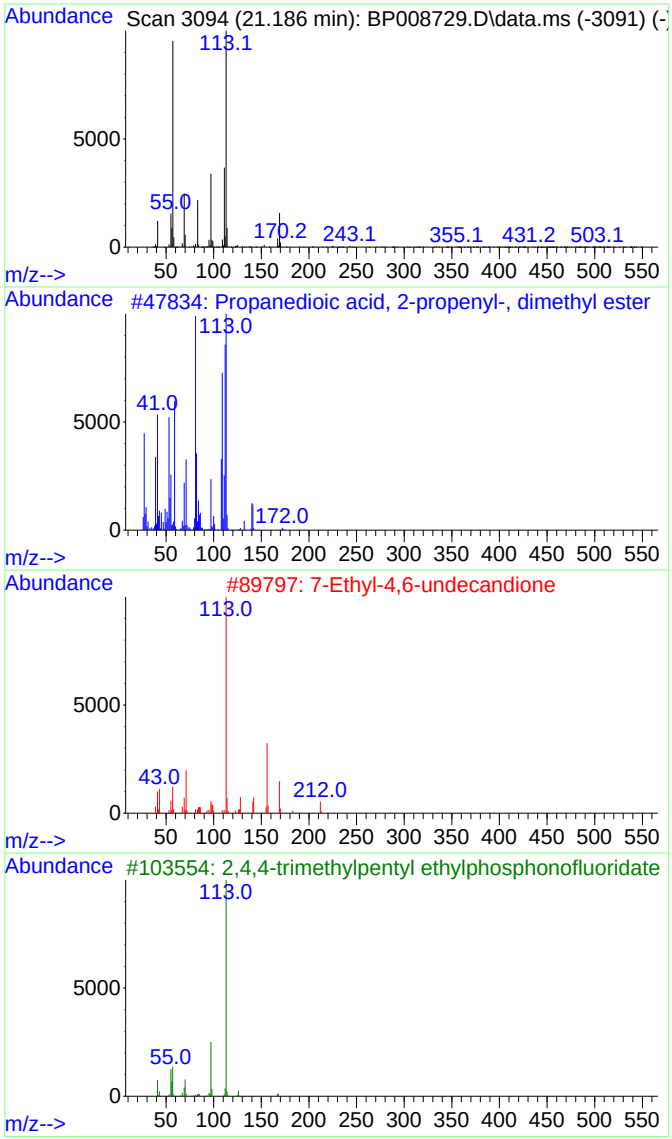
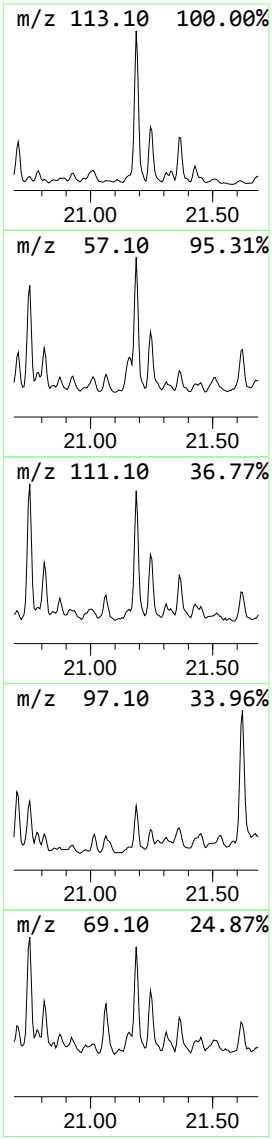
Peak Number 12 unknown21.186 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.186	8.88 ng	3320660	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanedioic acid, 2-propenyl-, ...	172	C8H12O4	040637-56-7	53
2	7-Ethyl-4,6-undecandione	212	C13H24O2	1000374-11-8	38
3	2,4,4-trimethylpentyl ethylphosp...	224	C10H22FO2P	333416-13-0	37
4	5-Nonanone, 2,2,8,8-tetramethyl-	198	C13H26O	005709-95-5	37
5	3-Heptadec-8-enyl-2,4,10-trioxa-...	378	C24H42O3	1000189-57-5	33





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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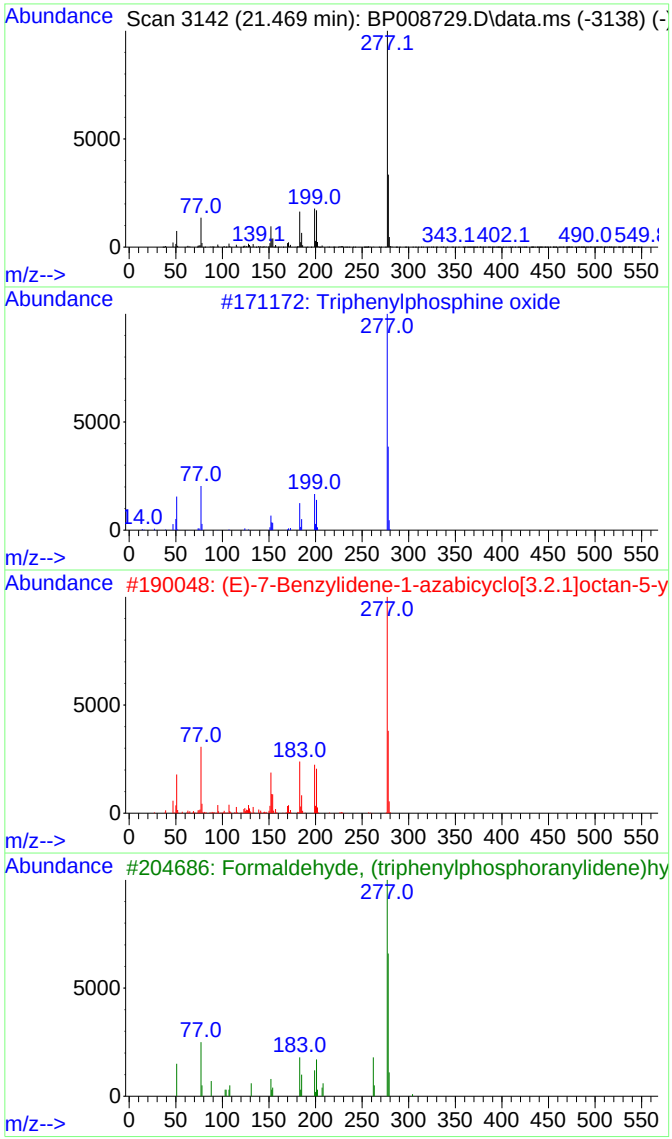
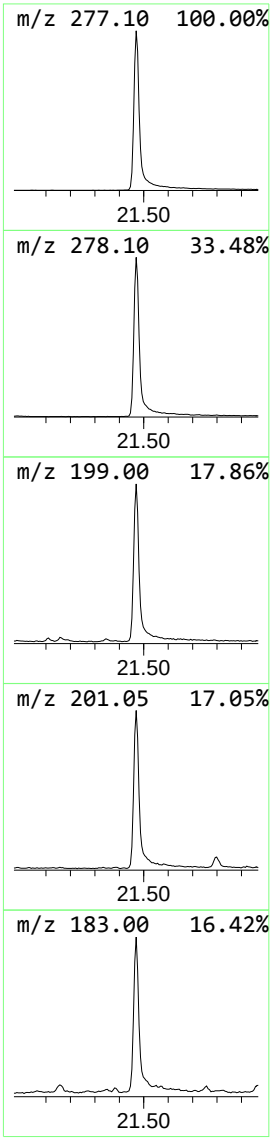
Peak Number 13 Triphenylphosphine oxide Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.469	6.85 ng	2560350	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	90
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	38
4	5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	38
5	Thiophene-3-carbonitrile, 4-(4-m...	277	C13H11NO2S2	1000268-75-0	33





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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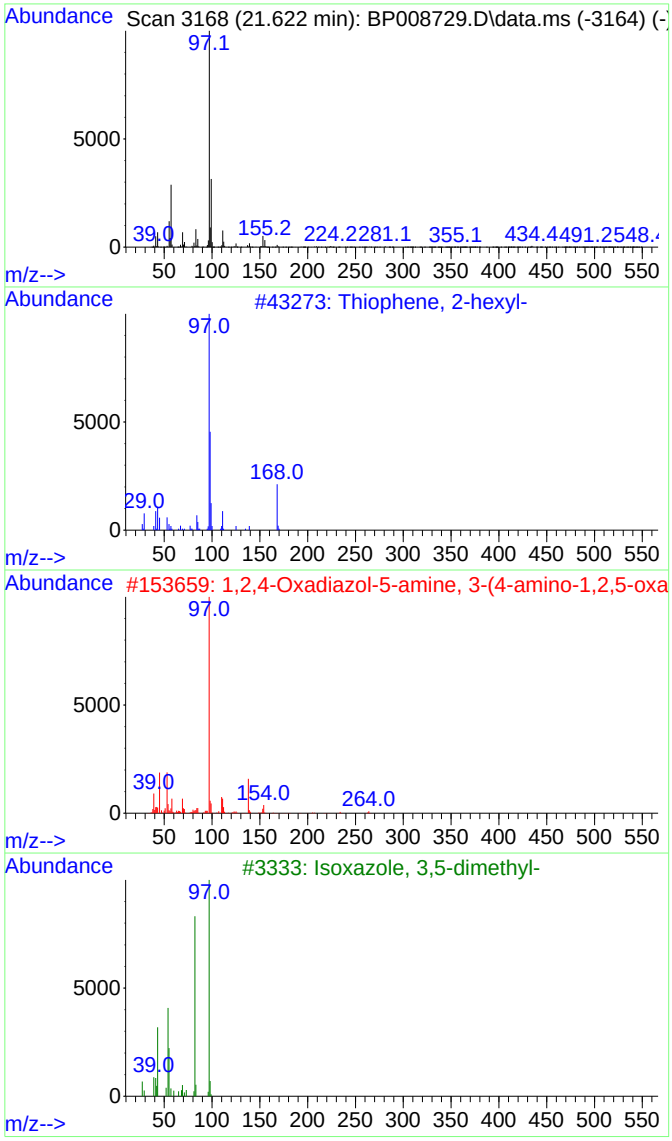
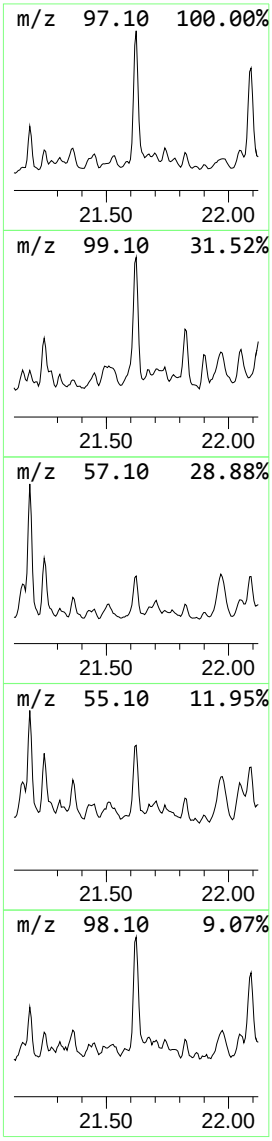
Peak Number 14 Thiophene, 2-hexyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.622	5.83 ng	2178840	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, 2-hexyl-	168	C10H16S	018794-77-9	59
2	1,2,4-Oxadiazol-5-amine, 3-(4-am...	264	C9H8N6O2S	1000351-26-9	50
3	Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	50
4	Sulfurous acid, cyclohexylmethyl...	416	C24H48O3S	1000309-22-5	38
5	Bis(2-isopropyl-5-methylcyclohex...	372	C21H41O3P	1000510-36-7	38





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TIC Library : C:\Database\NIST20.L
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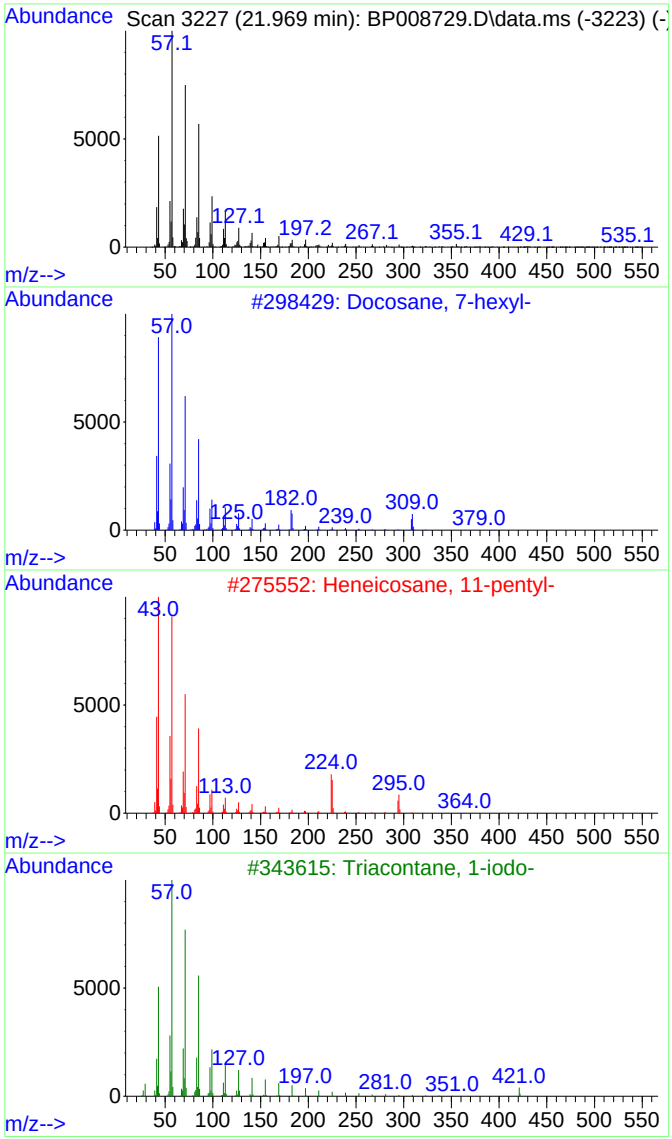
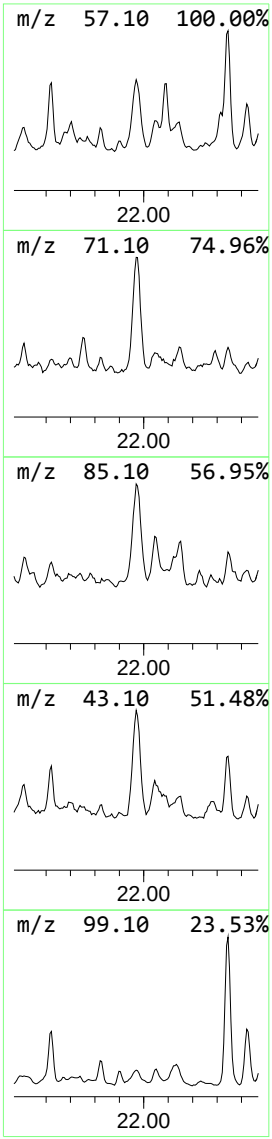
Peak Number 15 Docosane, 7-hexyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.969	6.94 ng	2596880	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 7-hexyl-	394	C28H58	055373-86-9	93
2	Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	91
3	Triacontane, 1-iodo-	548	C30H61I	1000406-32-3	91
4	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	91
5	Heptadecane	240	C17H36	000629-78-7	91





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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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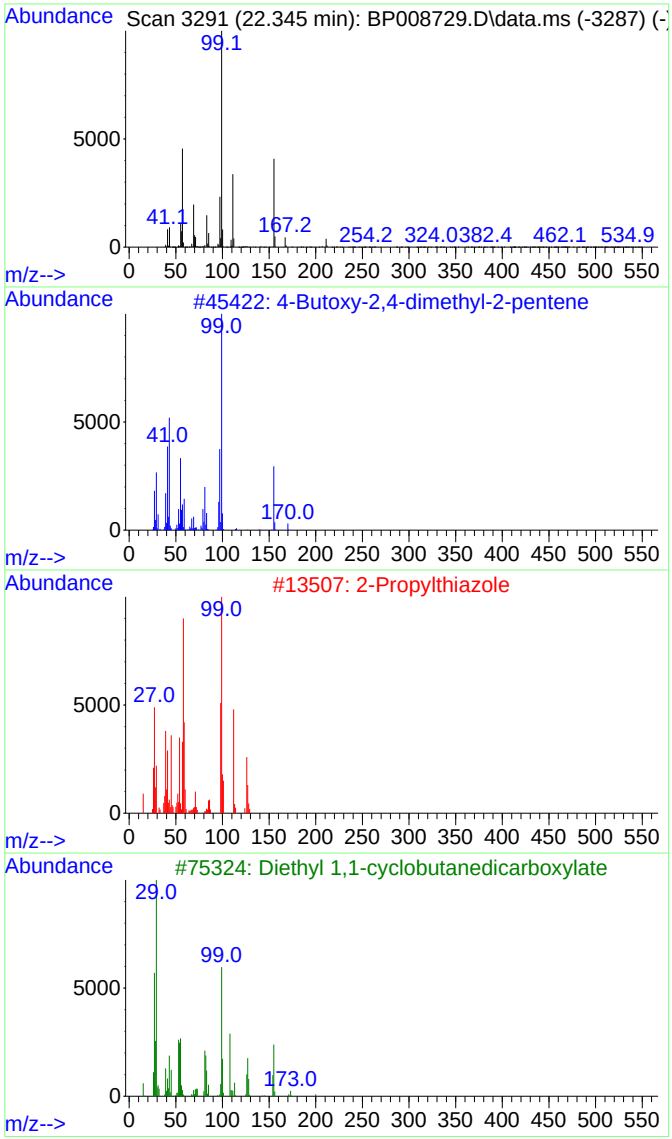
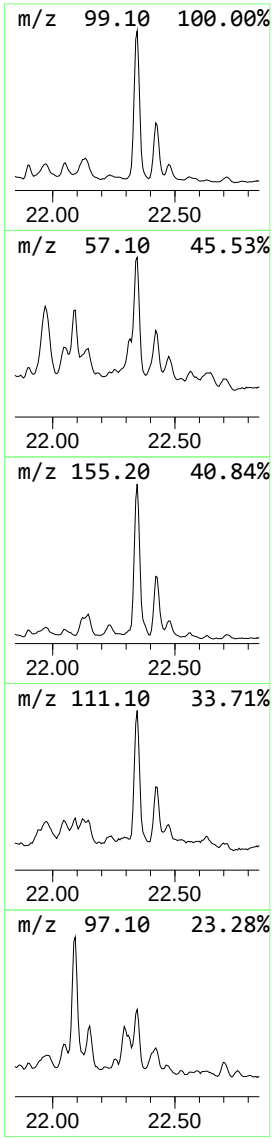
Peak Number 16 unknown22.345 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.345	10.60 ng	3962530	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	36
2	2-Propylthiazole	127	C6H9NS	017626-75-4	35
3	Diethyl 1,1-cyclobutanedicarboxy...	200	C10H16O4	003779-29-1	33
4	Hexanoic acid, 6-tridecyl ester	298	C19H38O2	1000279-29-5	32
5	4,4'-Bi-1,3,2-dioxaborolane, 2,2...	198	C8H16B2O4	062337-94-4	32





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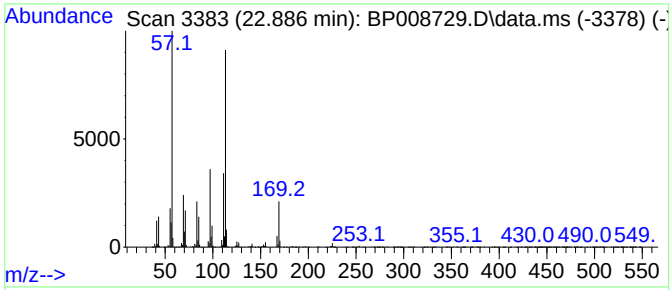
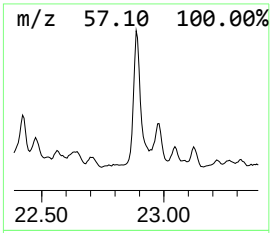
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

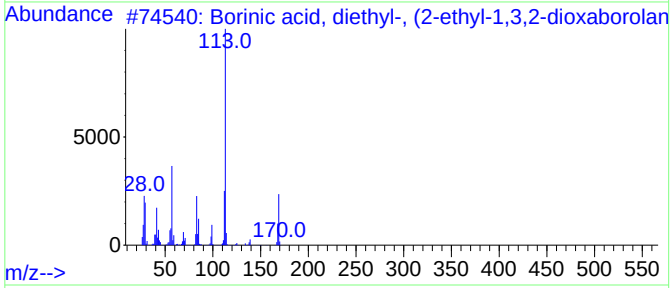
****
Peak Number 17 Borinic acid, diethyl-, (2-... Concentration Rank 5

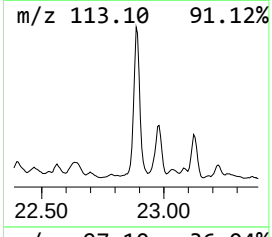
R.T.	EstConc	Area	Relative to ISTD	R.T.
22.886	16.17 ng	4536520	Perylene-d12	23.769

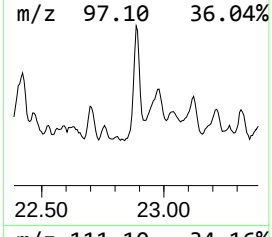
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Borinic acid, diethyl-, (2-ethyl...	198	C9H20B2O3	058163-56-7	53
2	Ribitol, 1,3:4,5-di-O-(ethylbora...	212	C9H18B2O4	1000149-52-8	47
3	Pyrazole, 3-nitro-	113	C3H3N3O2	026621-44-3	43
4	7-Ethyl-4,6-undecandione	212	C13H24O2	1000374-11-8	43
5	Dibutyl itaconate	242	C13H22O4	002155-60-4	40

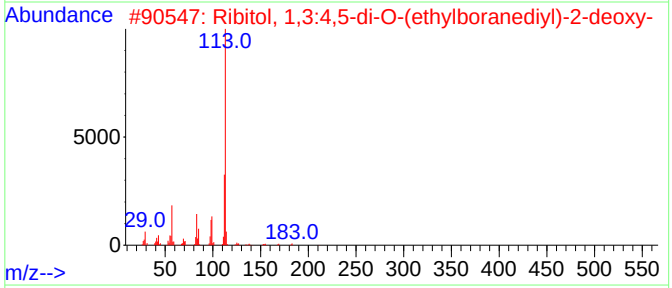


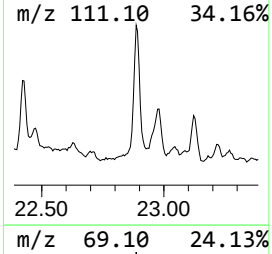


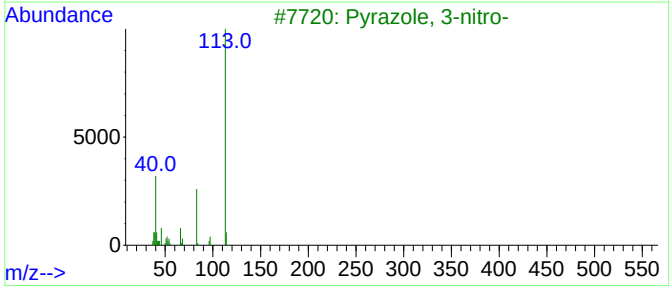


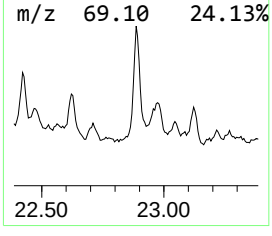












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008729.D
Acq On : 07 Jan 2022 16:49
Operator : CG/JU
Sample : N1049-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
7211979

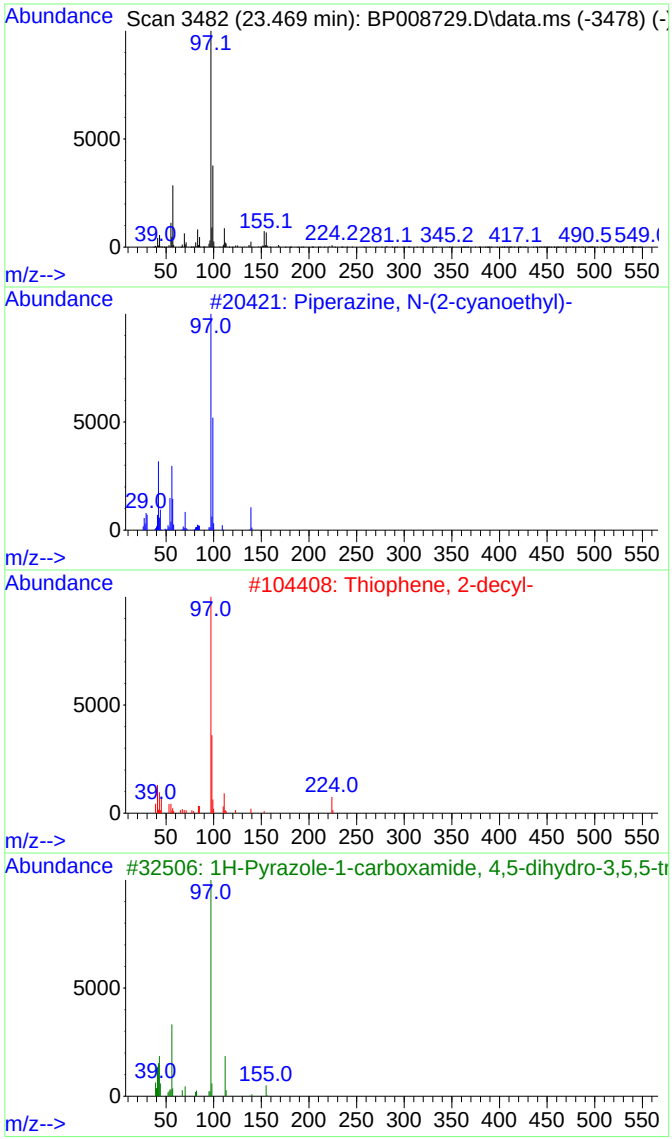
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

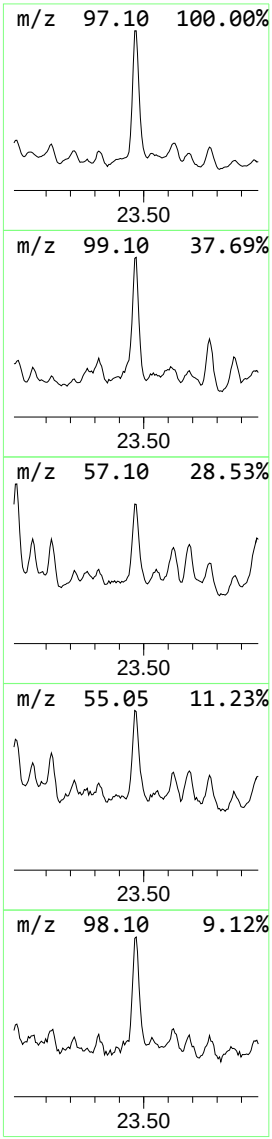
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 Piperazine, N-(2-cyanoethyl)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.469	7.34 ng	2058780	Perylene-d12	23.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Piperazine, N-(2-cyanoethyl)-	139	C7H13N3	1000325-03-2	64
2	Thiophene, 2-decyl-	224	C14H24S	024769-39-9	53
3	1H-Pyrazole-1-carboxamide, 4,5-d...	155	C7H13N3O	003786-02-5	53
4	Thiophene, 2-dodecyl-	252	C16H28S	004861-61-4	42
5	2-Pyrazoline, 1-isobutyl-3-methyl-	140	C8H16N2	026964-53-4	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008729.D
Acq On : 07 Jan 2022 16:49
Operator : CG/JU
Sample : N1049-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
7211979

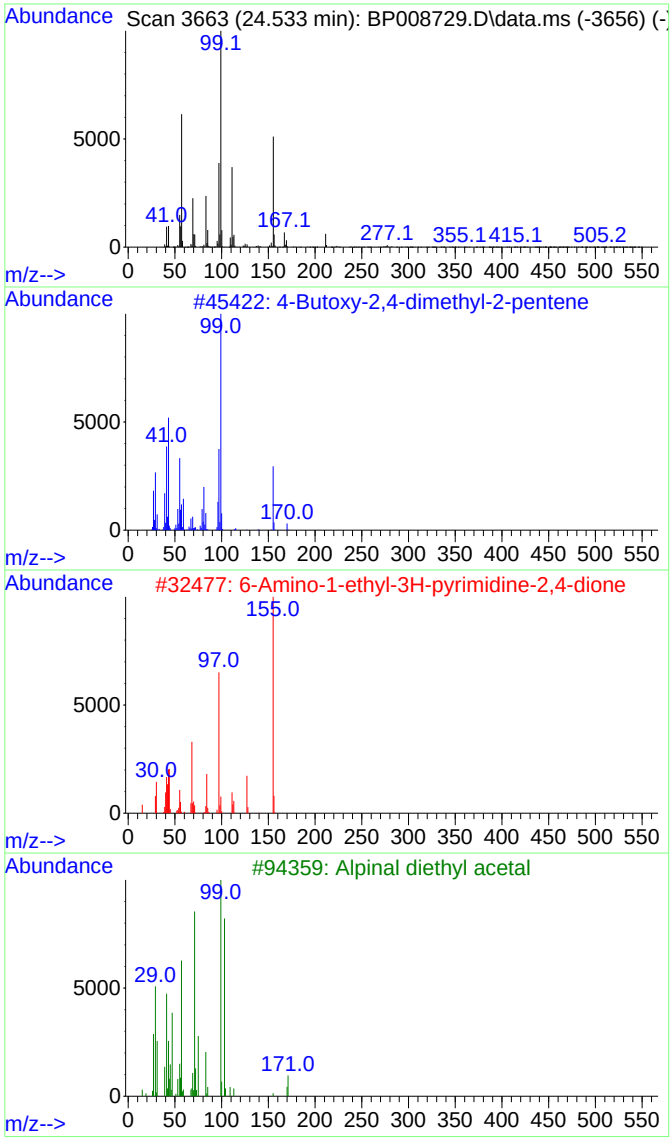
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

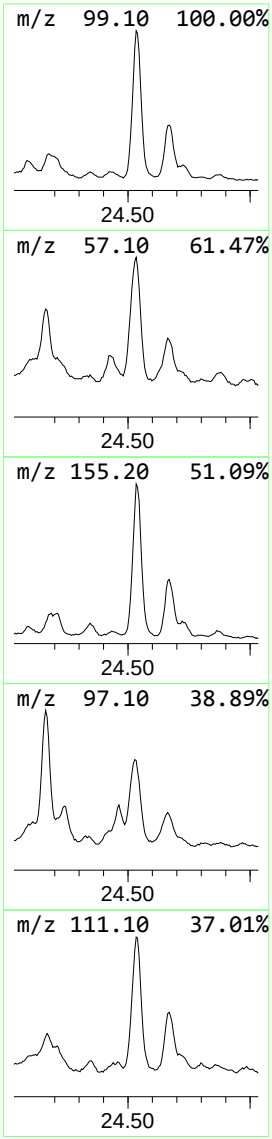
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 4-Butoxy-2,4-dimethyl-2-pen... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.533	17.66 ng	4955210	Perylene-d12	23.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	53
2	6-Amino-1-ethyl-3H-pyrimidine-2,...	155	C6H9N3O2	041862-09-3	38
3	Alpinal diethyl acetal	216	C13H28O2	1000430-79-8	35
4	2-Propylthiazole	127	C6H9NS	017626-75-4	25
5	Succinic acid, 4,4-dimethylpent-...	314	C18H34O4	1000381-71-8	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008729.D
Acq On : 07 Jan 2022 16:49
Operator : CG/JU
Sample : N1049-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
7211979

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

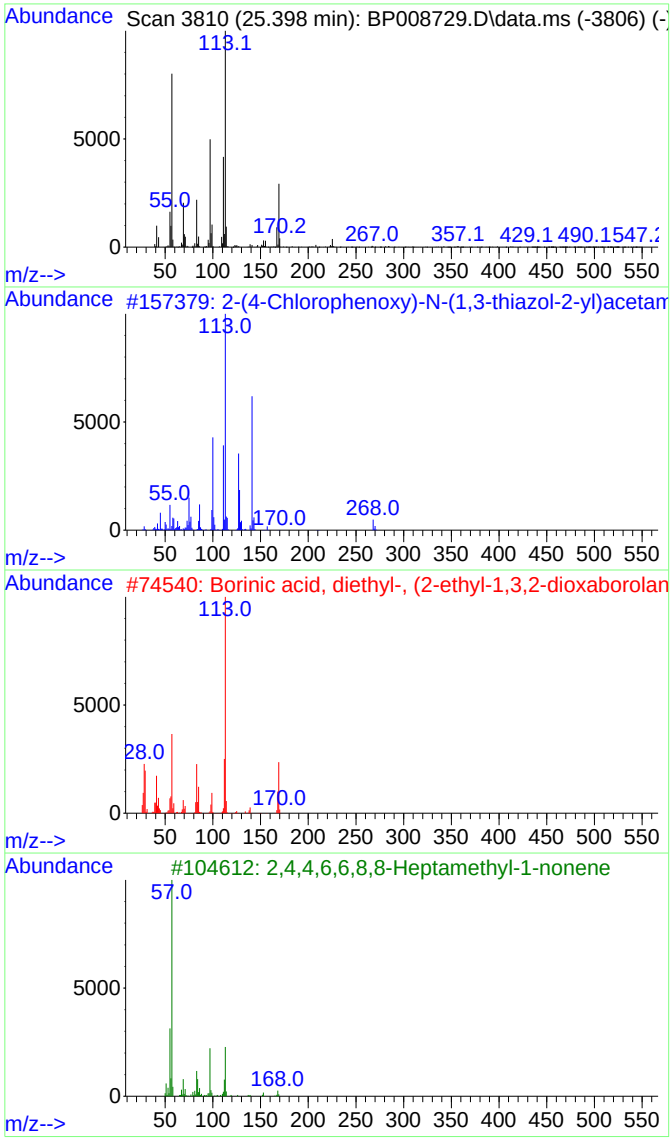
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

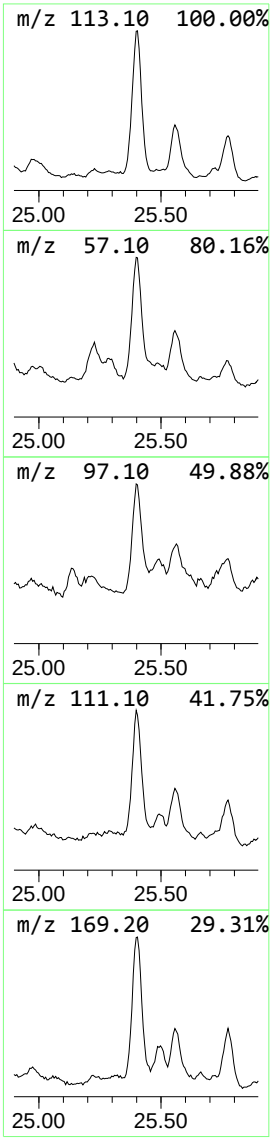
****

Peak Number 20 unknown25.398 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.398	6.29 ng	1764220	Perylene-d12	23.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(4-Chlorophenoxy)-N-(1,3-thiaz...	268	C11H9ClN2O2S	037666-22-1	43
2	Borinic acid, diethyl-, (2-ethyl...	198	C9H20B2O3	058163-56-7	37
3	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	37
4	1H-Pyrazole, 4-nitro-	113	C3H3N3O2	002075-46-9	35
5	1-Isopropyl-2-methylpropyl ethyl...	210	C9H20FO2P	1000298-33-2	32





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008729.D
Acq On : 07 Jan 2022 16:49
Operator : CG/JU
Sample : N1049-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
7211979

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.070	19.9	ng	2320460	1	7.869	2335230	20.0
Ethanol, 2-(2-b...	10.452	6.2	ng	802169	2	10.669	2608890	20.0
unknown13.575	13.575	5.8	ng	1050650	3	14.504	3650060	20.0
2(3H)-Furanone,...	16.663	11.5	ng	2648280	4	17.257	4592740	20.0
unknown17.351	17.351	6.8	ng	1565870	4	17.257	4592740	20.0
n-Hexadecanoic ...	18.163	18.0	ng	4126400	4	17.257	4592740	20.0
unknown18.986	18.986	17.4	ng	3990640	4	17.257	4592740	20.0
Hexanoic acid, ...	19.051	6.8	ng	1570310	4	17.257	4592740	20.0
Octadecanoic acid	19.392	11.2	ng	4180850	5	21.345	7478790	20.0
Propanedioic ac...	19.510	5.9	ng	2219420	5	21.345	7478790	20.0
unknown20.751	20.751	9.7	ng	3615370	5	21.345	7478790	20.0
unknown21.186	21.186	8.9	ng	3320660	5	21.345	7478790	20.0
Triphenylphosph...	21.469	6.8	ng	2560350	5	21.345	7478790	20.0
Thiophene, 2-he...	21.622	5.8	ng	2178840	5	21.345	7478790	20.0
Docosane, 7-hexyl-	21.969	6.9	ng	2596880	5	21.345	7478790	20.0
unknown22.345	22.345	10.6	ng	3962530	5	21.345	7478790	20.0
Borinic acid, d...	22.886	16.2	ng	4536520	6	23.769	5611330	20.0
Piperazine, N-(...	23.469	7.3	ng	2058780	6	23.769	5611330	20.0
4-Butoxy-2,4-di...	24.533	17.7	ng	4955210	6	23.769	5611330	20.0
unknown25.398	25.398	6.3	ng	1764220	6	23.769	5611330	20.0