LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060725.D
Acq On : 1 Apr 2024 21:37
Operator : MA/JU
Sample : P1915-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-A-COMP

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_G\Methods\8270-BG032924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060725.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.102	12	19	26	rBV3	35793	82175	1.64%	0.198%
2	3.173	26	31	45	rVB	476487	717716	14.30%	1.733%
3	3.684	113	118	130	rBV	93547	147845	2.95%	0.357%
4	5.535	425	433	443	rBV	1394668	2199262	43.81%	5.311%
5	7.115	692	702	711	rBV	1649221	2777224	55.33%	6.706%
6	7.955	838	845	851	rBV	312204	514037	10.24%	1.241%
7	9.107	1033	1041	1048	rBV	950209	1612826	32.13%	3.895%
8	9.677	1130	1138	1146	rVB3	30050	55847	1.11%	0.135%
9	10.529	1276	1283	1290	rBV	117572	191010	3.81%	0.461%
10	10.752	1311	1321	1327	rBV	467024	835498	16.64%	2.018%
11	11.492	1440	1447	1455	rBV3	34056	67159	1.34%	0.162%
12	12.409	1598	1603	1611	rVB3	31043	59851	1.19%	0.145%
13	13.214	1732	1740	1749	rVB	2175897	3456173	68.85%	8.346%
14	13.431	1771	1777	1782	rBV3	33670	52415	1.04%	0.127%
15	14.095	1881	1890	1893	rBV3	27910	51172	1.02%	0.124%
16	14.136	1894	1897	1906	rVB6	28837	62563	1.25%	0.151%
17	14.506	1955	1960	1964	rBV	52679	76288	1.52%	0.184%
18	14.583	1964	1973	1979	rBV	757987	1217083	24.25%	2.939%
19	14.642	1979	1983	1991	rVB	81416	141078	2.81%	0.341%
20	14.800	2003	2010	2011	rBV4	50876	81344	1.62%	0.196%
21	14.976	2033	2040	2050	rBV2	63246	144233	2.87%	0.348%
22	15.200	2074	2078	2083	rVV6	27708	55879	1.11%	0.135%
23	15.458	2118	2122	2126	rBV	66115	88338	1.76%	0.213%
24	15.629	2146	2151	2156	rBV	95551	144159	2.87%	0.348%
25	15.870	2185	2192	2197	rBV	54136	112554	2.24%	0.272%
26	16.069	2219	2226	2235	rVB	1896979	2817339	56.13%	6.803%
27	16.322	2265	2269	2272	rBV	85463	124954	2.49%	0.302%
28	16.351	2272	2274	2280	rVB2	100596	120850	2.41%	0.292%
29	16.974	2378	2380	2387	rVB3	48471	75245	1.50%	0.182%
30	17.098	2397	2401	2407	rBV2	121587	242334	4.83%	0.585%
31	17.174	2412	2414	2417	rVB	63096	63565	1.27%	0.153%
32	17.327	2435	2440	2444	rBV	850880	1347496	26.84%	3.254%
33	17.374	2444	2448	2454	rVB	992400	1456495	29.02%	3.517%
34	17.462	2459	2463	2468	rVB	207463	305496	6.09%	0.738%
35	17.726	2504	2508	2513	rVB	101920	149276	2.97%	0.360%
36	17.861	2527	2531	2535	rVB2	90137	107864	2.15%	0.260%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060725.D
Acq On : 1 Apr 2024 21:37
Operator : MA/JU
Sample : P1915-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-A-COMP

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_G\Methods\8270-BG032924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	18.208	2587	2590	2593	rBV	99971	132138	2.63%	0.319%
38	18.249	2593	2597	2604	rVB2	460498	725029	14.44%	1.751%
39	18.396	2618	2622	2627	rBV2	184647	335237	6.68%	0.810%
40	18.549	2646	2648	2653	rVB3	72185	89430	1.78%	0.216%
41	18.707	2672	2675	2678	rBV	77836	108212	2.16%	0.261%
42	18.737	2678	2680	2690	rVB2	93614	124984	2.49%	0.302%
43	19.183	2753	2756	2760	rBV2	89982	99872	1.99%	0.241%
44	19.260	2765	2769	2772	rBV2	66403	99695	1.99%	0.241%
45	19.383	2785	2790	2797	rVB	1488971	2093191	41.70%	5.055%
46	19.518	2810	2813	2818	rBV2	110909	151137	3.01%	0.365%
47	19.741	2842	2851	2860	rBV	1248034	2365357	47.12%	5.712%
48	19.959	2879	2888	2898	rVB	3542956	5019697	100.00%	12.122%
49	20.071	2903	2907	2912	rBV4	97555	230186	4.59%	0.556%
50	20.241	2933	2936	2940	rVB2	178374	232987	4.64%	0.563%
51	20.341	2950	2953	2957	rVB	87057	105491	2.10%	0.255%
52	20.394	2960	2962	2966	rVB2	134234	162549	3.24%	0.393%
53	20.582	2991	2994	2997	rBV2	79911	97837	1.95%	0.236%
54	21.281	3109	3113	3118	rBV3	349344	474925	9.46%	1.147%
55	21.528	3150	3155	3158	rBV	690826	926686	18.46%	2.238%
56	21.586	3158	3165	3170	rVV2	1110632	2718230	54.15%	6.564%
57	21.639	3170	3174	3182	rVB	577291	984743	19.62%	2.378%
58	22.808	3369	3373	3378	rVB2	209704	331265	6.60%	0.800%
59	23.743	3527	3532	3540	rBV	322180	939695	18.72%	2.269%
60	24.736	3694	3701	3709	rVB2	437537	1108212	22.08%	2.676%

Sum of corrected areas: 41411428

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Data File : BG060725.D
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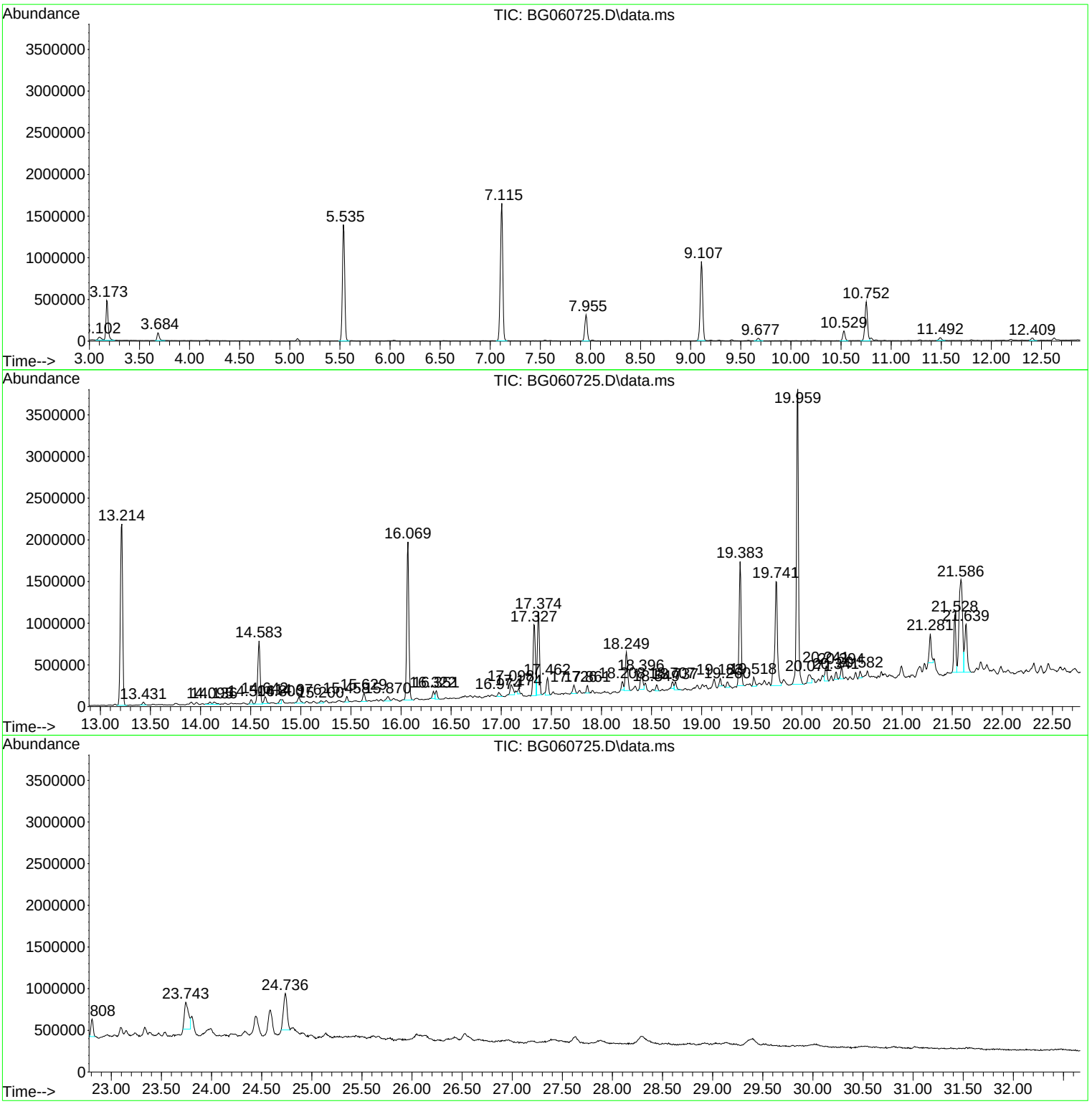
Operator : MA/JU
Sample : P1915-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-A-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.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_G\Data\BG040124\
Data File : BG060725.D
Acq On : 1 Apr 2024 21:37
Operator : MA/JU
Sample : P1915-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-A-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

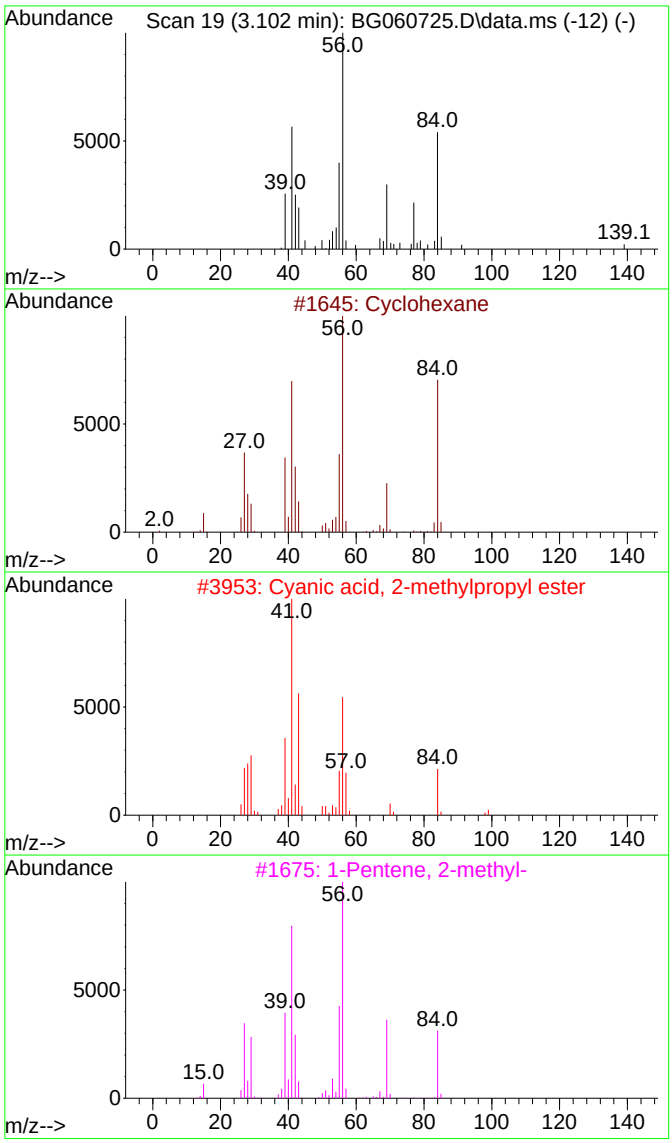
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

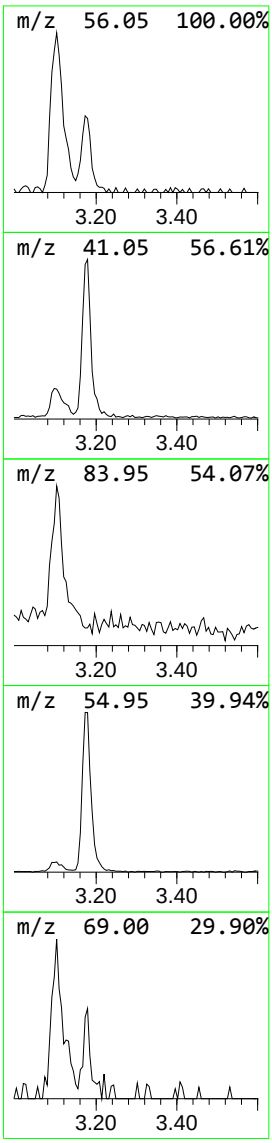
****

Peak Number 1 Cyclohexane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.102	3.20 ng	82175	1,4-Dichlorobenzene-d4	7.955

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	87
2	Cyanic acid, 2-methylpropyl ester	99	C5H9NO	001768-25-8	72
3	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64
4	Cyclopentane, methyl-	84	C6H12	000096-37-7	45
5	Cyclopropane, 1-ethyl-1-methyl-	84	C6H12	053778-43-1	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060725.D
Acq On : 1 Apr 2024 21:37
Operator : MA/JU
Sample : P1915-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-A-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

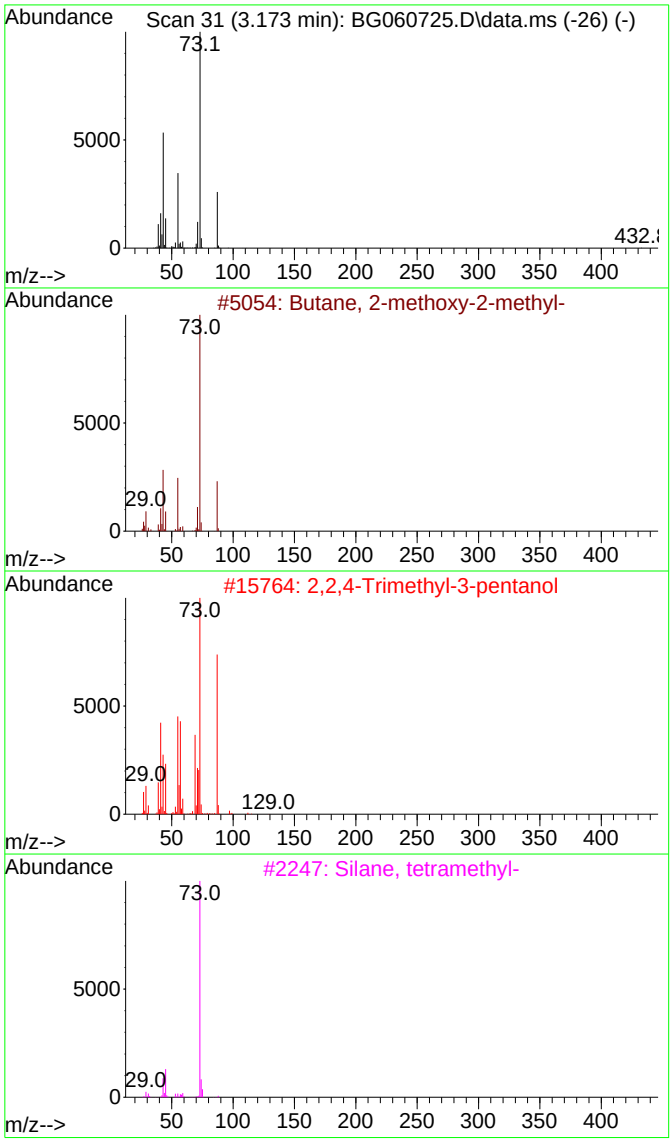
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

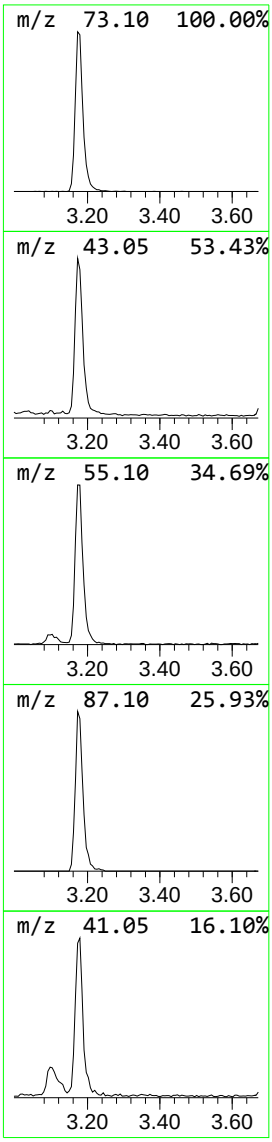
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.173	27.92 ng	717716	1,4-Dichlorobenzene-d4	7.955

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	38
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5	2-OXOPROPIONAMIDE	87	C3H5NO2	000631-66-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060725.D
Acq On : 1 Apr 2024 21:37
Operator : MA/JU
Sample : P1915-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-A-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

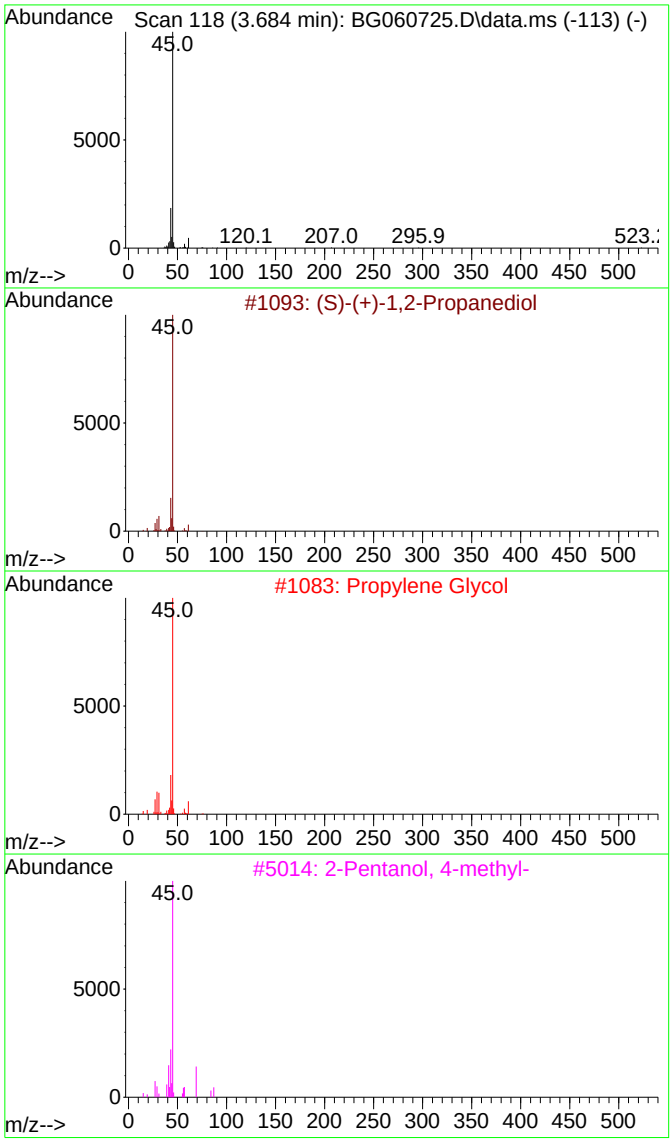
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

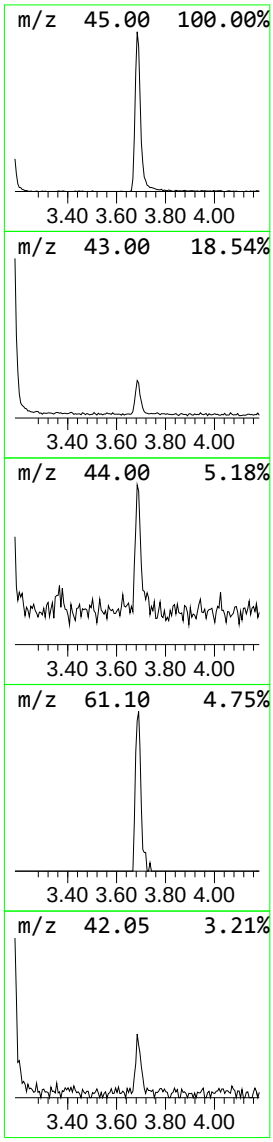
****

Peak Number 3 (S)-(+)-1,2-Propanediol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.684	5.75 ng	147845	1,4-Dichlorobenzene-d4	7.955

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	Propylene Glycol	76	C3H8O2	000057-55-6	9
3	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	9
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060725.D
Acq On : 1 Apr 2024 21:37
Operator : MA/JU
Sample : P1915-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-A-COMP

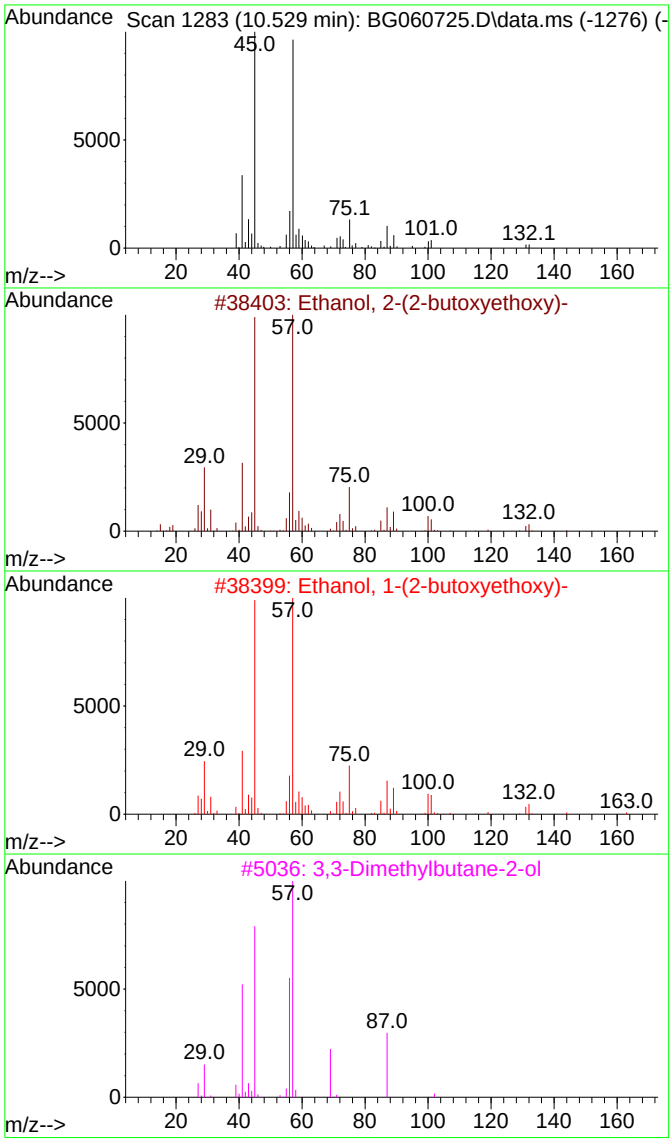
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

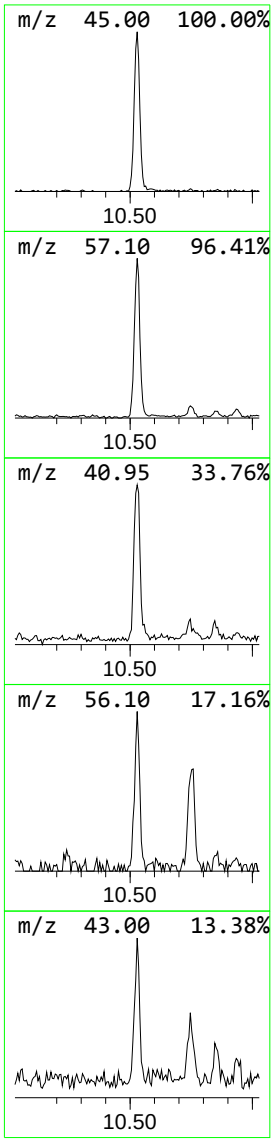
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.529	4.57 ng	191010	Naphthalene-d8	10.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	72
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
4	Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	50
5	Butyl lactate	146	C7H14O3	000138-22-7	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060725.D
Acq On : 1 Apr 2024 21:37
Operator : MA/JU
Sample : P1915-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-A-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

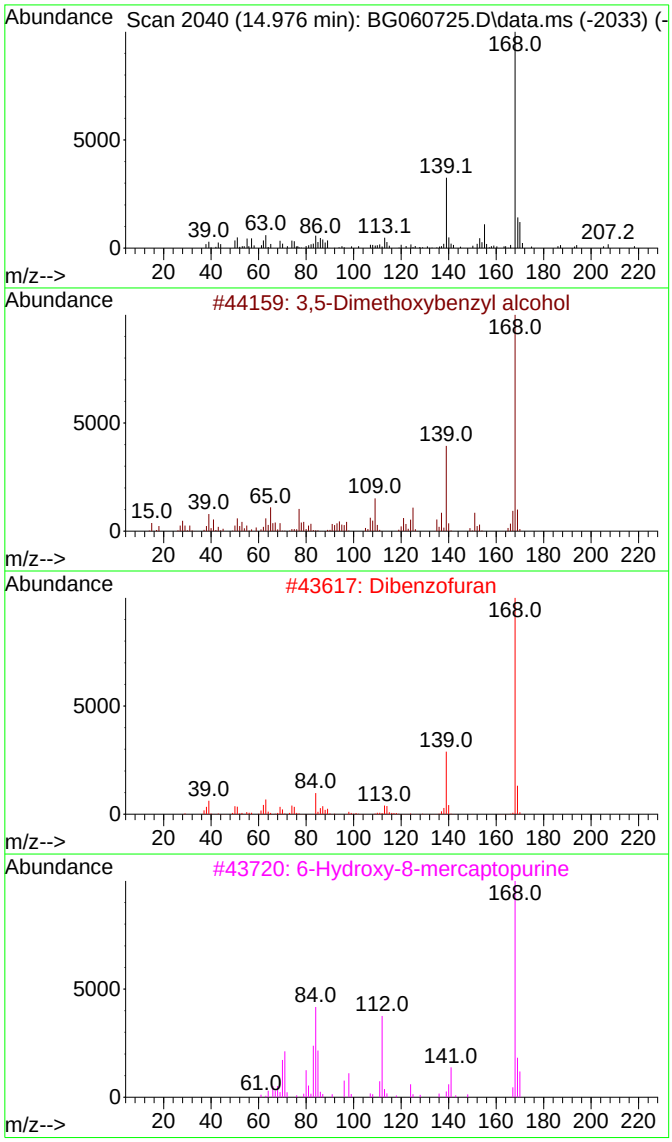
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

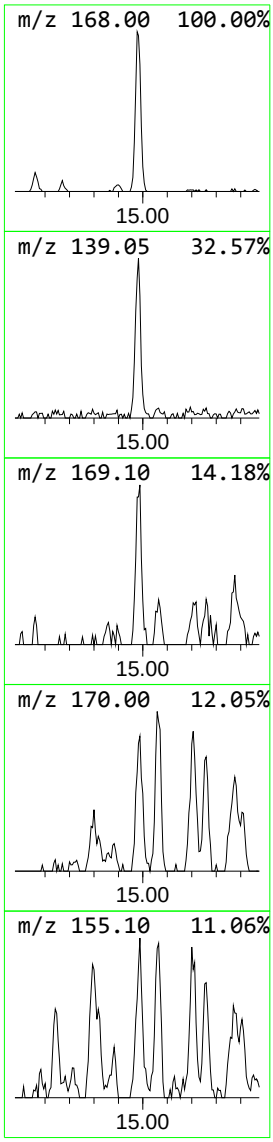
****

Peak Number 6 3,5-Dimethoxybenzyl alcohol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.977	2.37 ng	144233	Acenaphthene-d10	14.583

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Dimethoxybenzyl alcohol	168	C9H12O3	000705-76-0	64
2	Dibenzofuran	168	C12H8O	000132-64-9	59
3	6-Hydroxy-8-mercaptopurine	168	C5H4N4OS	006305-94-8	53
4	Benzonitrile, 4-(pyrrol-1-yl)-	168	C11H8N2	023351-07-7	50
5	9H-Pyrido[3,4-b]indole	168	C11H8N2	000244-63-3	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
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Acq On : 1 Apr 2024 21:37
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Sample : P1915-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-A-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

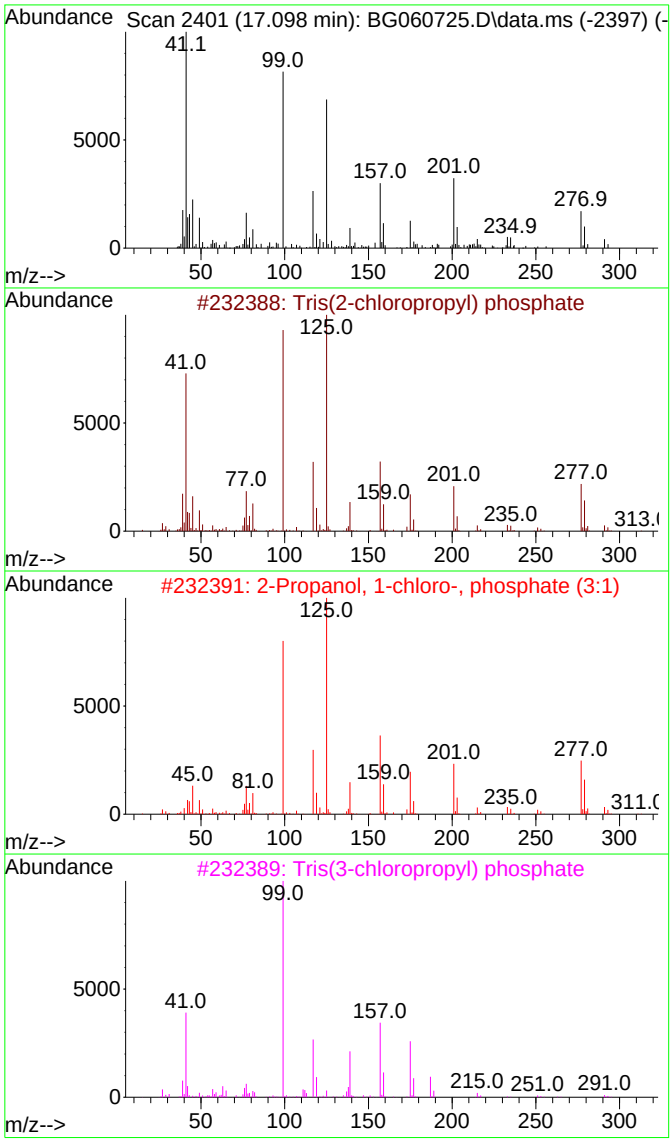
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

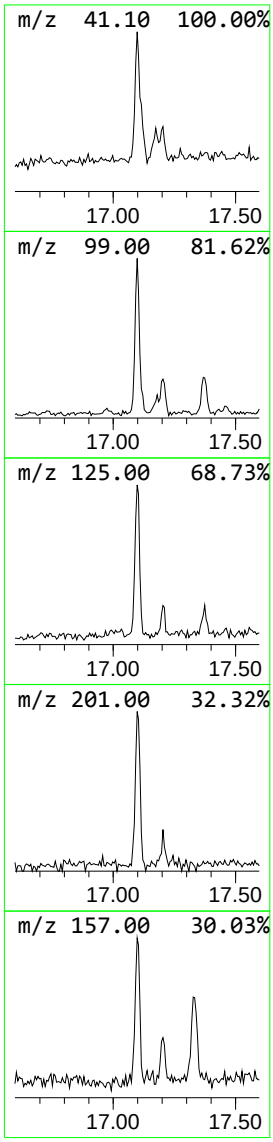
****

Peak Number 7 Tris(2-chloropropyl) phosphate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.098	3.60 ng	242334	Phenanthrene-d10	17.327

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tris(2-chloropropyl) phosphate	326	C9H18Cl3O4P	006145-73-9	86
2	2-Propanol, 1-chloro-, phosphate...	326	C9H18Cl3O4P	013674-84-5	50
3	Tris(3-chloropropyl) phosphate	326	C9H18Cl3O4P	001067-98-7	37
4	Bis(1-chloro-2-propyl)(3-chloro-...	326	C9H18Cl3O4P	137909-40-1	27
5	N-(3-Fluoro-phenyl)-2-piperazin-...	237	C12H16FN3O	1000484-49-3	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060725.D
Acq On : 1 Apr 2024 21:37
Operator : MA/JU
Sample : P1915-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-A-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

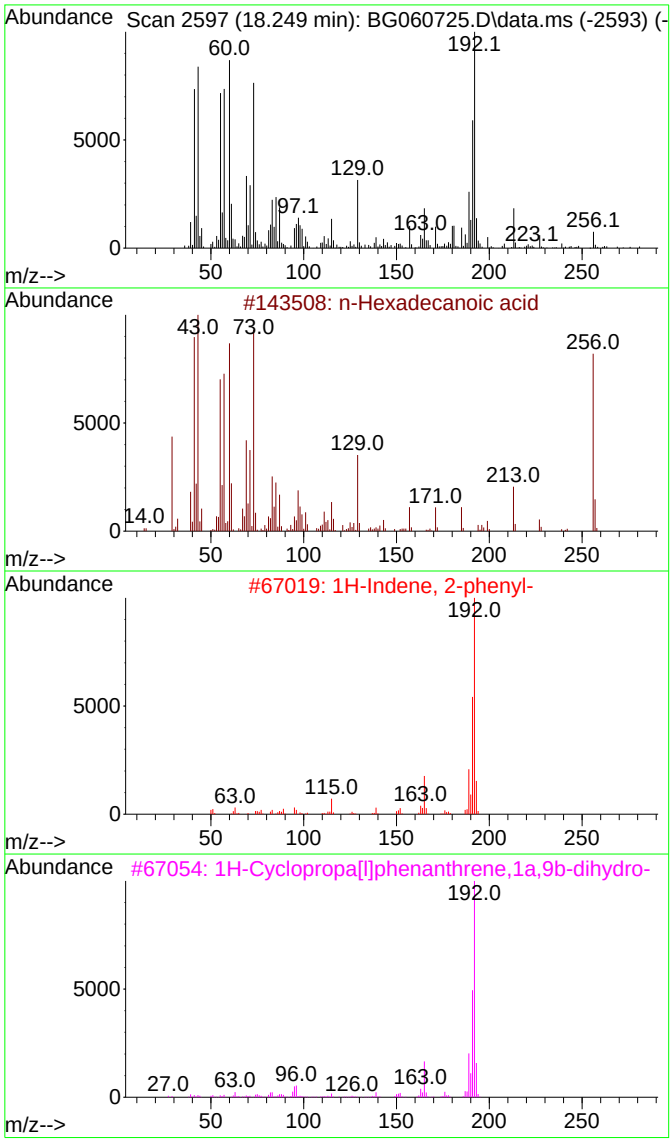
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

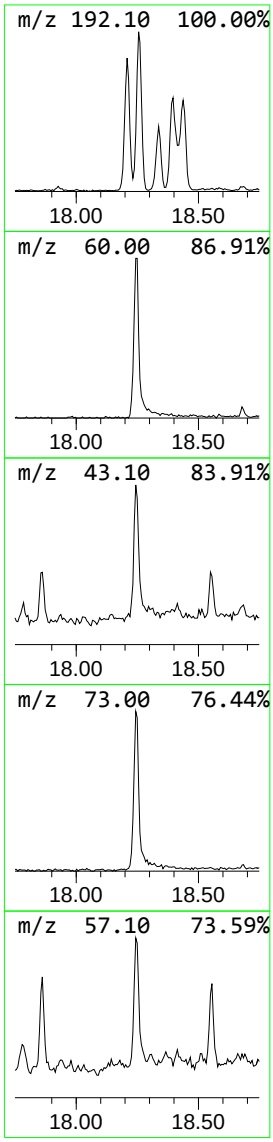
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.249	10.76 ng	725029	Phenanthrene-d10	17.327

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	74
3	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	70
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	70
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060725.D
Acq On : 1 Apr 2024 21:37
Operator : MA/JU
Sample : P1915-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-A-COMP

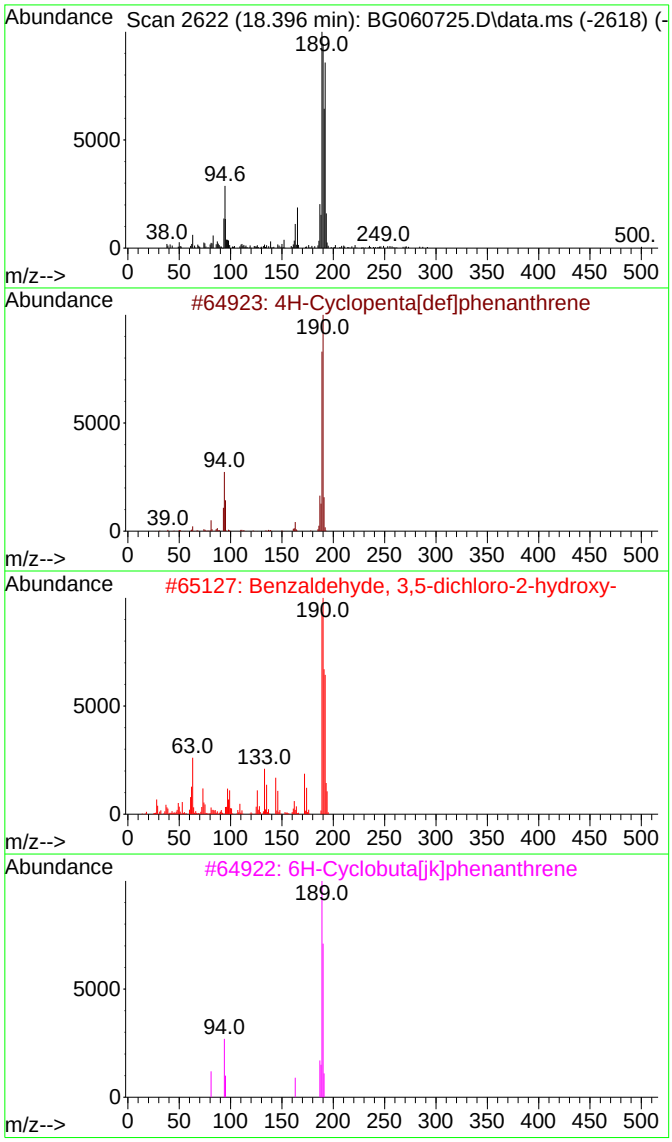
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

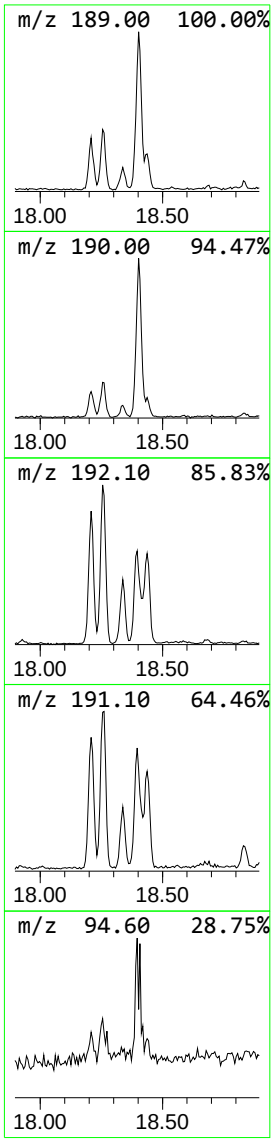
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.396	4.98 ng	335237	Phenanthrene-d10	17.327

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	64
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	38
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060725.D
Acq On : 1 Apr 2024 21:37
Operator : MA/JU
Sample : P1915-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-A-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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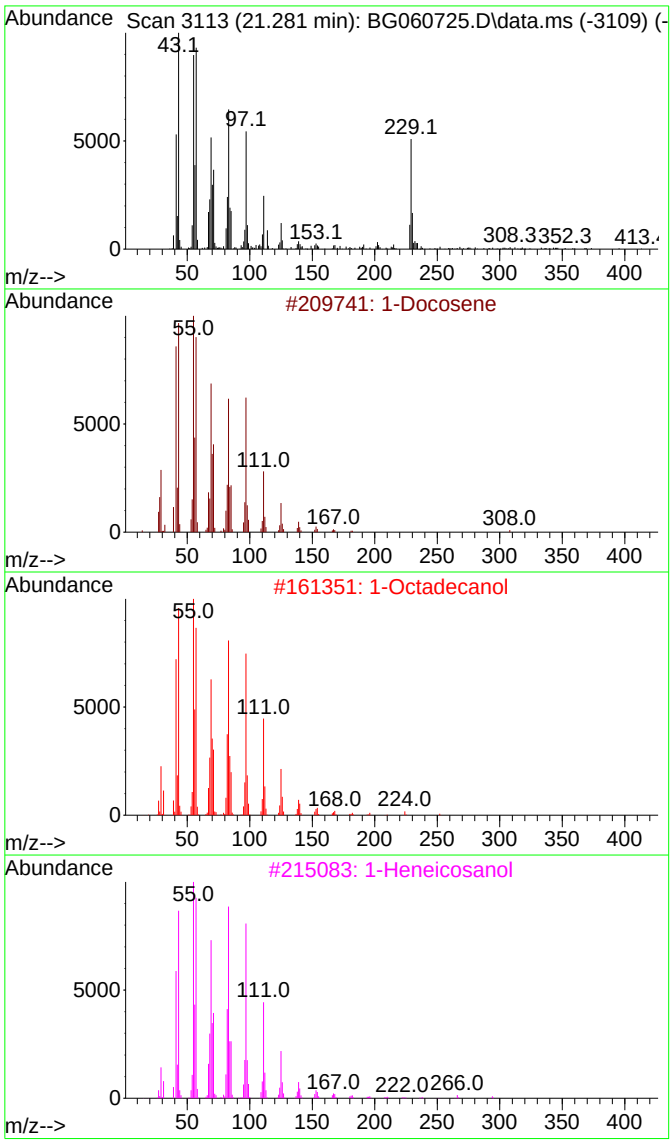
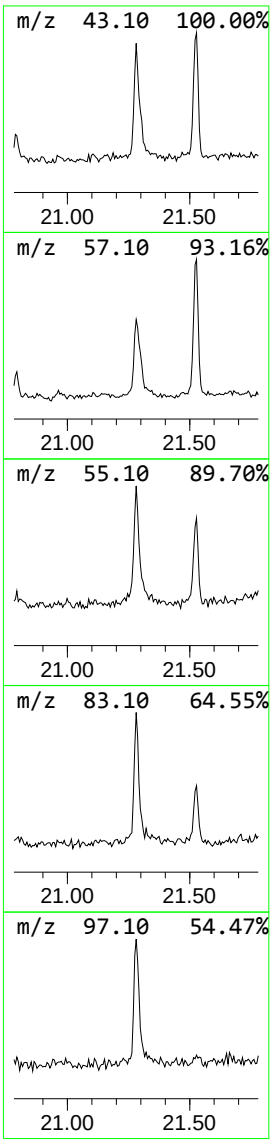
****

Peak Number 10 1-Docosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.281	3.49 ng	474925	Chrysene-d12	21.592

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	1-Octadecanol	270	C18H38O	000112-92-5	70
3	1-Heneicosanol	312	C21H44O	015594-90-8	70
4	1-Hexadecanol	242	C16H34O	036653-82-4	70
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060725.D
Acq On : 1 Apr 2024 21:37
Operator : MA/JU
Sample : P1915-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-A-COMP

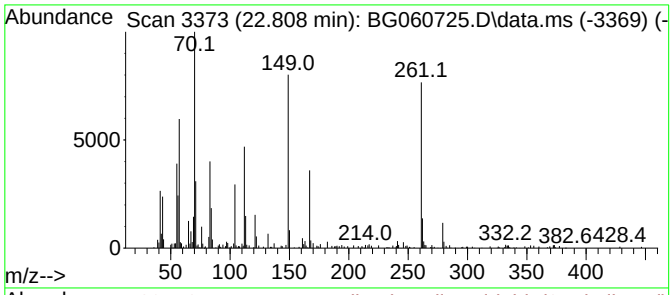
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

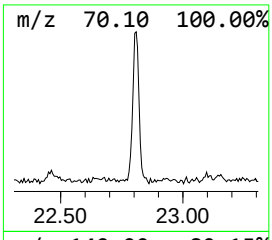
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

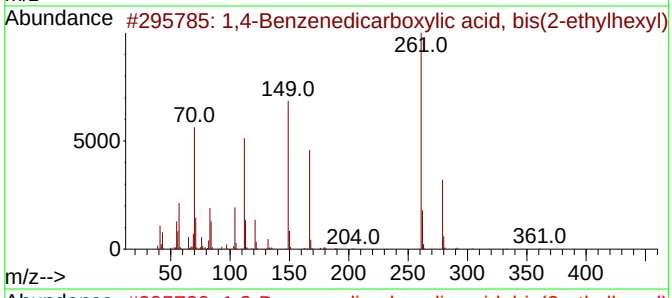
****
Peak Number 11 1,4-Benzenedicarboxylic aci... Concentration Rank 9

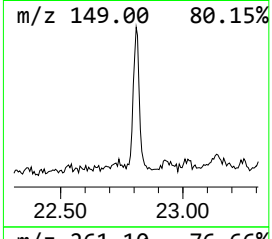
R.T.	EstConc	Area	Relative to ISTD	R.T.
22.808	2.44 ng	331265	Chrysene-d12	21.592

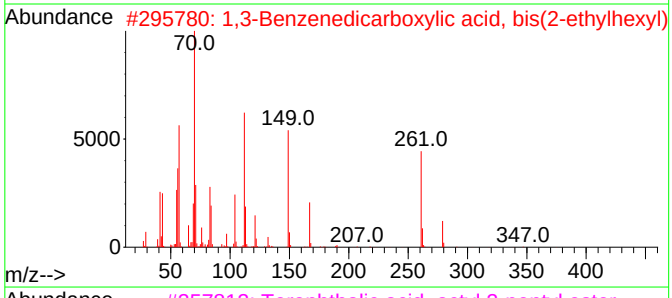
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	64
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	58
3	Terephthalic acid, octyl 2-penty...	348	C21H32O4	1000323-55-2	25
4	9-(2',2'-Dimethylpropanoilhydraz...	576	C30H42Cl2N4O3	1000111-04-6	22
5	Acetic acid, cyano-, 2-ethylhexy...	197	C11H19NO2	013361-34-7	22

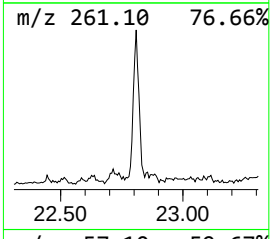


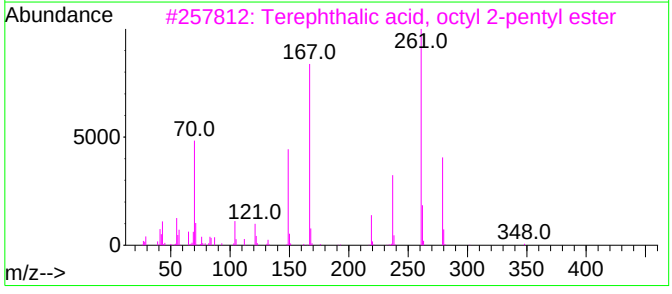


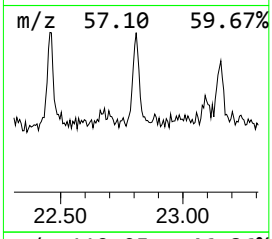


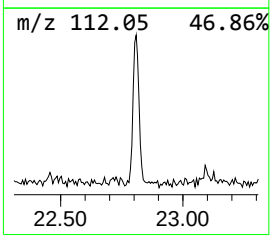












Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060725.D
Acq On : 1 Apr 2024 21:37
Operator : MA/JU
Sample : P1915-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-A-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.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
Cyclohexane	3.102	3.2	ng	82175	1	7.955	514037	20.0
Butane, 2-metho...	3.173	27.9	ng	717716	1	7.955	514037	20.0
(S)-(+)-1,2-Pro...	3.684	5.8	ng	147845	1	7.955	514037	20.0
Ethanol, 2-(2-b...	10.529	4.6	ng	191010	2	10.752	835498	20.0
3,5-Dimethoxybe...	14.977	2.4	ng	144233	3	14.583	1217080	20.0
Tris(2-chloropr...	17.098	3.6	ng	242334	4	17.327	1347500	20.0
n-Hexadecanoic ...	18.249	10.8	ng	725029	4	17.327	1347500	20.0
4H-Cyclopenta[d...	18.396	5.0	ng	335237	4	17.327	1347500	20.0
1-Docosene	21.281	3.5	ng	474925	5	21.592	2718230	20.0
1,4-Benzenedica...	22.808	2.4	ng	331265	5	21.592	2718230	20.0