LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020122\
Data File : BP008991.D
Acq On : 01 Feb 2022 17:37
Operator : CG/JU
Sample : N1340-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-6(1.5-2)

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-BP011422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008991.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.034	4	8	17	rVB	294512	422480	4.31%	0.617%
2	4.028	172	177	184	rVB	72321	109167	1.11%	0.160%
3	4.952	328	334	343	rVB	100629	179978	1.84%	0.263%
4	5.417	406	413	420	rBV	2866866	4436355	45.25%	6.482%
5	7.011	672	684	702	rBV	2607407	4822170	49.18%	7.046%
6	7.828	815	823	832	rBV	755855	1327706	13.54%	1.940%
7	8.987	1012	1020	1029	rBV	1848670	3259070	33.24%	4.762%
8	9.416	1084	1093	1099	rBV	57853	99079	1.01%	0.145%
9	10.622	1290	1298	1304	rBV	984791	1772453	18.08%	2.590%
10	10.675	1304	1307	1314	rVB	77323	135415	1.38%	0.198%
11	12.293	1569	1582	1591	rBV	104134	194987	1.99%	0.285%
12	12.510	1613	1619	1627	rBV	78168	133225	1.36%	0.195%
13	13.087	1709	1717	1737	rBV	4991840	7797404	79.53%	11.393%
14	13.299	1747	1753	1760	rBV3	106658	160887	1.64%	0.235%
15	13.787	1831	1836	1841	rBV	73848	122980	1.25%	0.180%
16	14.463	1943	1951	1958	rBV	1461438	2428988	24.77%	3.549%
17	14.528	1958	1962	1971	rVB3	85897	189576	1.93%	0.277%
18	14.869	2015	2020	2027	rBV	78062	120635	1.23%	0.176%
19	15.516	2124	2130	2133	rBV2	80679	134911	1.38%	0.197%
20	15.816	2175	2181	2188	rVB3	51520	101248	1.03%	0.148%
21	15.963	2199	2206	2218	rBV	3404773	5430715	55.39%	7.935%
22	16.192	2241	2245	2254	rBV4	71980	165909	1.69%	0.242%
23	16.881	2358	2362	2368	rBV3	69179	126183	1.29%	0.184%
24	16.987	2370	2380	2385	rVV6	66209	195400	1.99%	0.286%
25	17.040	2386	2389	2398	rVB2	74224	130945	1.34%	0.191%
26	17.222	2414	2420	2424	rBV	1929620	2760663	28.16%	4.034%
27	17.263	2424	2427	2435	rVV	891875	1318054	13.44%	1.926%
28	17.357	2438	2443	2448	rVB	172374	277180	2.83%	0.405%
29	17.422	2449	2454	2459	rBV2	52392	98477	1.00%	0.144%
30	17.540	2472	2474	2482	rVB3	72150	112023	1.14%	0.164%
31	17.634	2486	2490	2498	rVV	74776	140979	1.44%	0.206%
32	17.804	2516	2519	2529	rVB2	84684	144119	1.47%	0.211%
33	18.092	2564	2568	2570	rBV	218024	297942	3.04%	0.435%
34	18.122	2570	2573	2574	rBV	248429	272209	2.78%	0.398%
35	18.275	2595	2599	2604	rBV2	213359	383838	3.91%	0.561%
36	18.316	2604	2606	2612	rVB	125752	149064	1.52%	0.218%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020122\
Data File : BP008991.D
Acq On : 01 Feb 2022 17:37
Operator : CG/JU
Sample : N1340-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-6(1.5-2)

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-BP011422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	18.575	2646	2650	2654	rBV	144173	212892	2.17%	0.311%
38	18.628	2656	2659	2667	rVB4	78466	149432	1.52%	0.218%
39	18.863	2696	2699	2703	rBV	83937	103907	1.06%	0.152%
40	18.981	2715	2719	2723	rBV	156014	234150	2.39%	0.342%
41	19.116	2738	2742	2748	rBV3	75502	155867	1.59%	0.228%
42	19.234	2757	2762	2769	rBV	1548238	2115956	21.58%	3.092%
43	19.351	2776	2782	2791	rVV3	179101	368623	3.76%	0.539%
44	19.586	2813	2822	2831	rVB	1228416	2088125	21.30%	3.051%
45	19.663	2831	2835	2842	rBV2	98342	158778	1.62%	0.232%
46	19.786	2850	2856	2861	rBV	8093105	9804938	100.00%	14.326%
47	19.898	2871	2875	2883	rBV4	109128	258595	2.64%	0.378%
48	20.069	2901	2904	2910	rVB2	211399	326976	3.33%	0.478%
49	20.169	2918	2921	2925	rBV	165640	211505	2.16%	0.309%
50	20.810	3027	3030	3035	rVB	117805	155288	1.58%	0.227%
51	21.039	3065	3069	3074	rVB3	445551	721809	7.36%	1.055%
52	21.092	3074	3078	3086	rVB2	474879	641484	6.54%	0.937%
53	21.222	3098	3100	3104	rVB	296791	314496	3.21%	0.460%
54	21.316	3109	3116	3120	rVV2	2446968	4228208	43.12%	6.178%
55	21.351	3120	3122	3131	rVB	713774	937030	9.56%	1.369%
56	21.433	3133	3136	3139	rVV2	180348	210174	2.14%	0.307%
57	22.986	3396	3400	3406	rBV	531699	1147349	11.70%	1.676%
58	23.616	3503	3507	3516	rVB	511298	945768	9.65%	1.382%
59	23.722	3519	3525	3532	rBV2	1471790	2997320	30.57%	4.379%

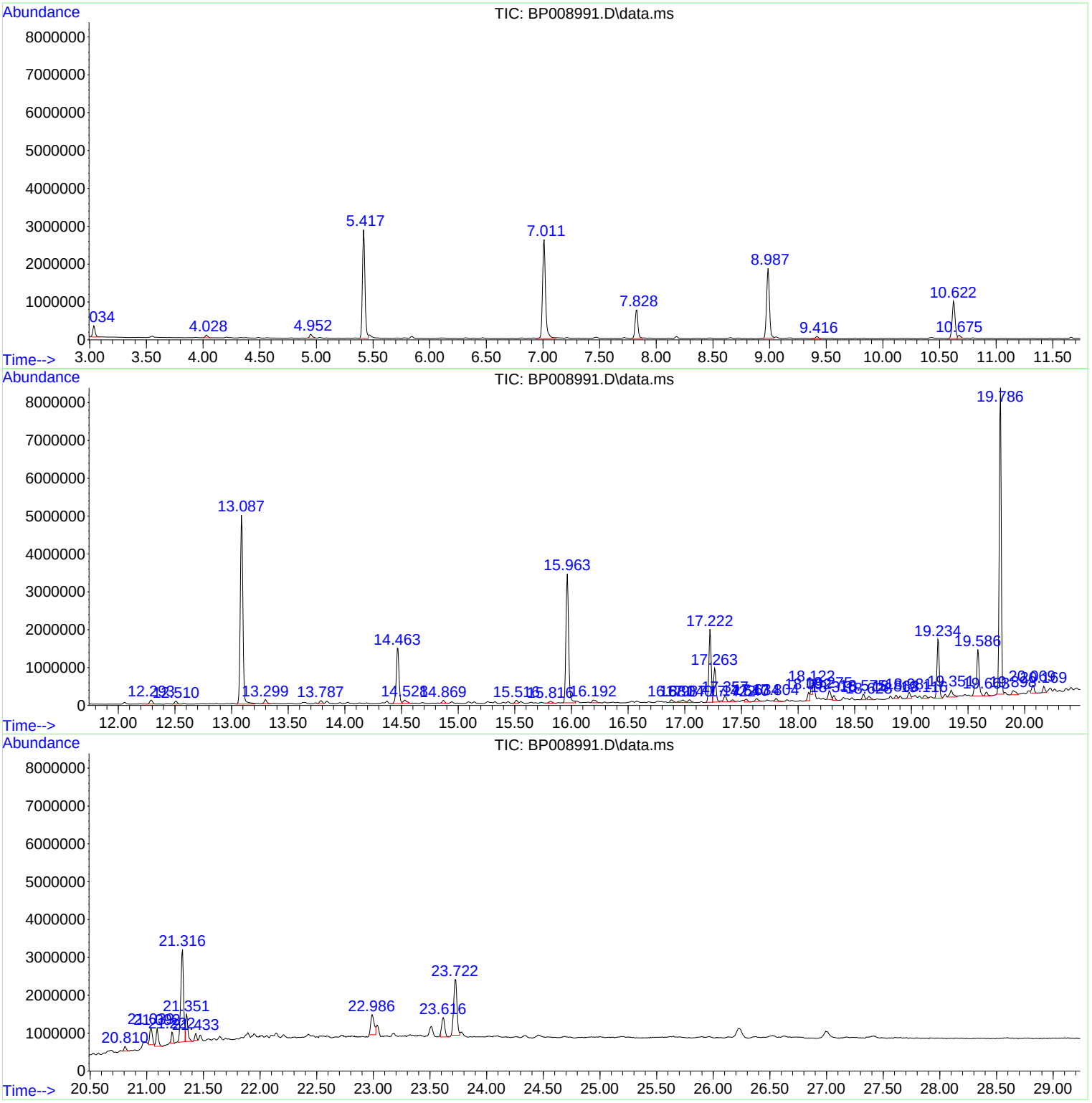
Sum of corrected areas: 68441084

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020122\
Data File : BP008991.D
Acq On : 01 Feb 2022 17:37
Operator : CG/JU
Sample : N1340-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-6(1.5-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP011422.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\BP020122\
Data File : BP008991.D
Acq On : 01 Feb 2022 17:37
Operator : CG/JU
Sample : N1340-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-6(1.5-2)

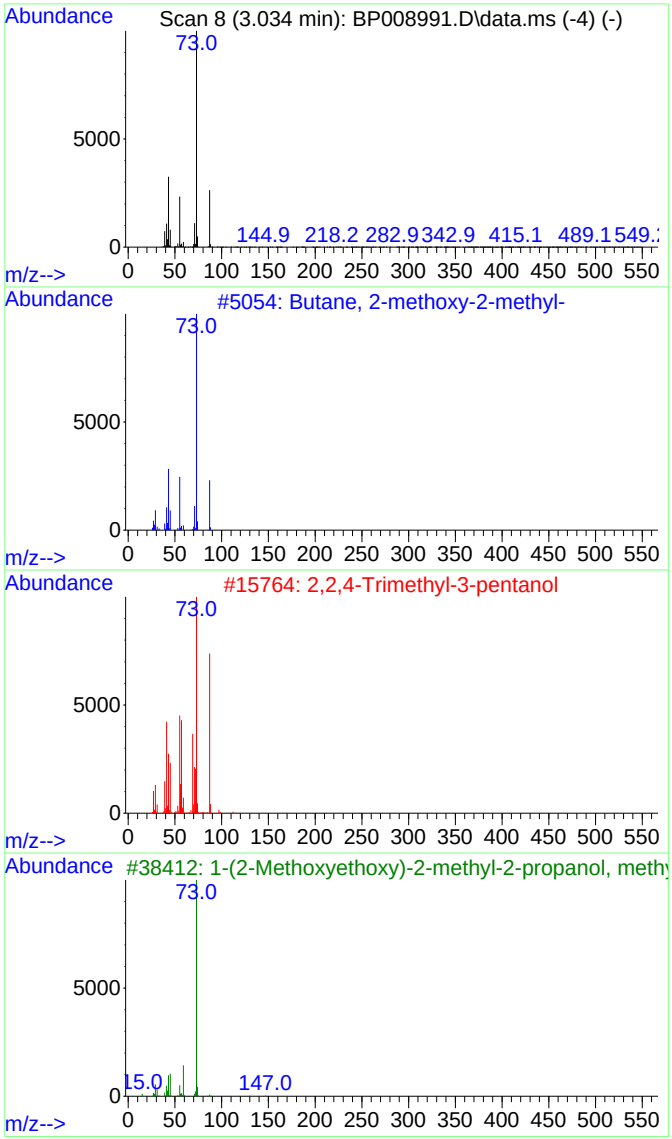
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP011422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

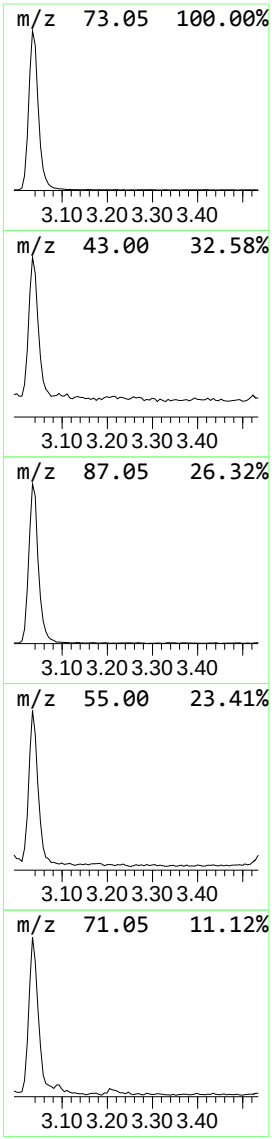
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.034	6.36 ng	422480	1,4-Dichlorobenzene-d4	7.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020122\
Data File : BP008991.D
Acq On : 01 Feb 2022 17:37
Operator : CG/JU
Sample : N1340-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-6(1.5-2)

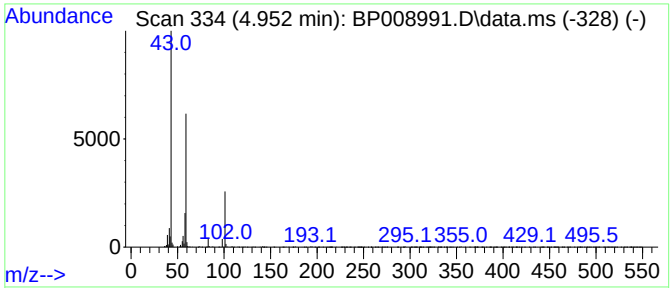
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP011422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

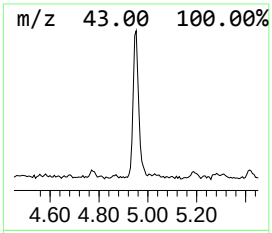
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

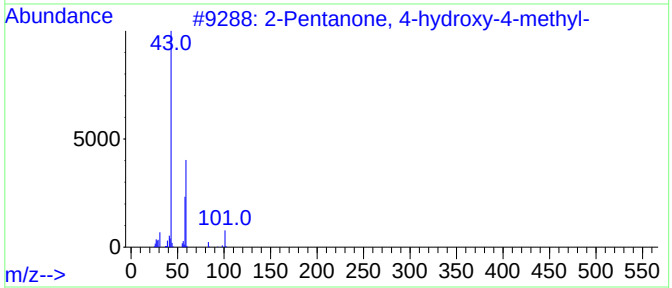
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

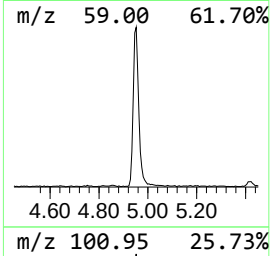
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.952	2.71 ng	179978	1,4-Dichlorobenzene-d4	7.828

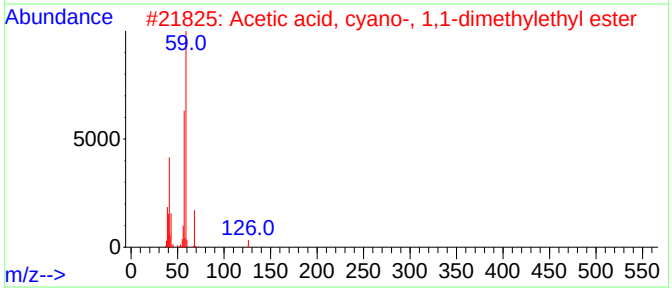
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Hexanamide	115	C6H13NO	000628-02-4	12
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	12

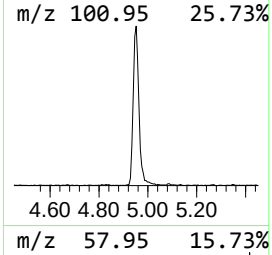


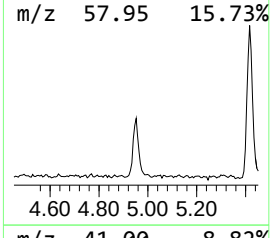


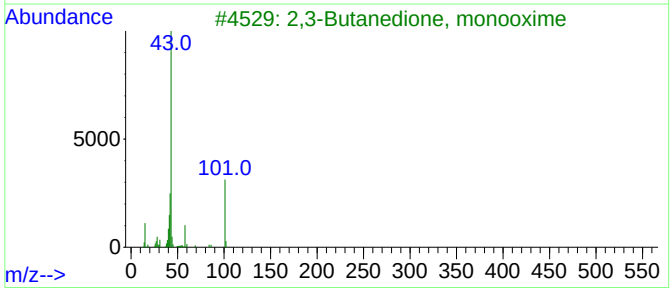


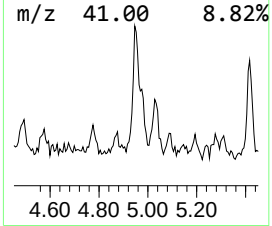












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020122\
Data File : BP008991.D
Acq On : 01 Feb 2022 17:37
Operator : CG/JU
Sample : N1340-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-6(1.5-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP011422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

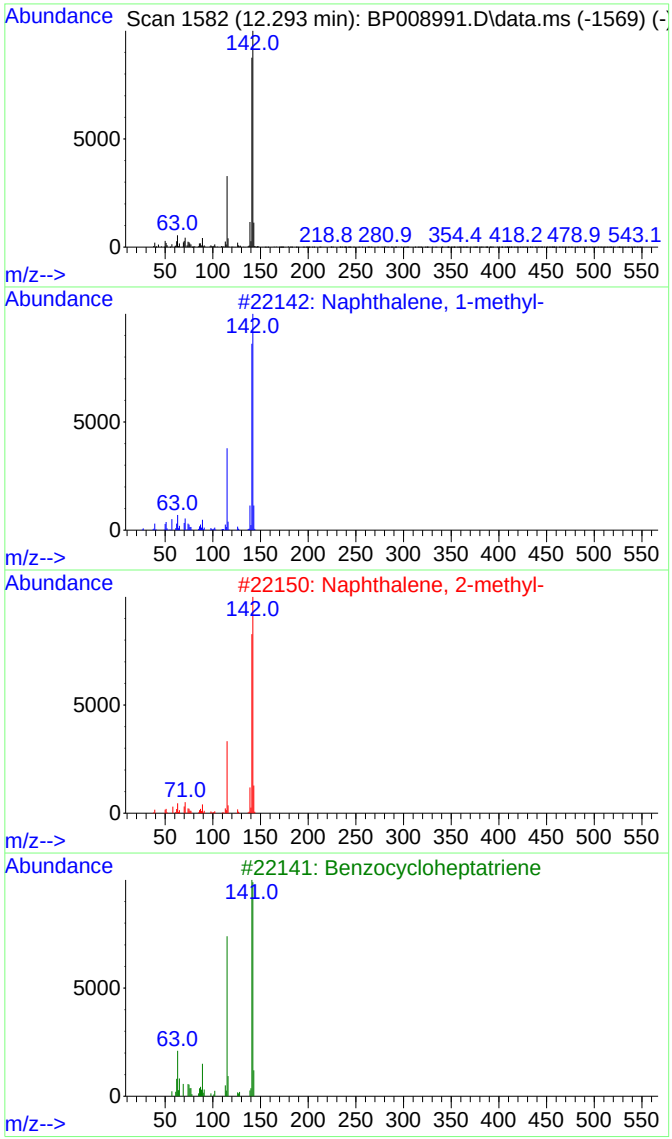
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

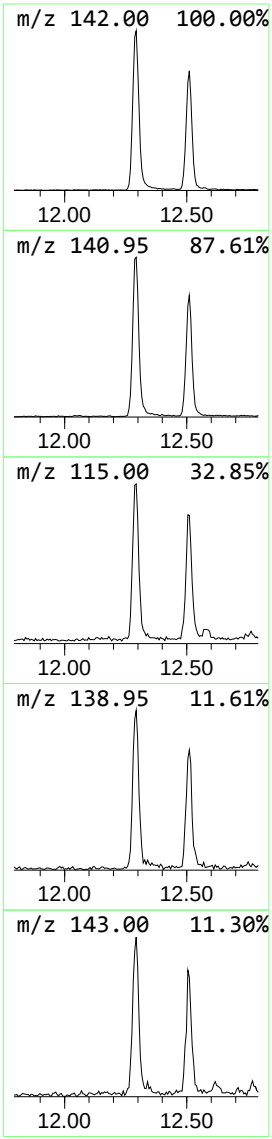
****

Peak Number 3 Benzocycloheptatriene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.293	2.20 ng	194987	Naphthalene-d8	10.622

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3	Benzocycloheptatriene	142	C11H10	000264-09-5	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020122\
Data File : BP008991.D
Acq On : 01 Feb 2022 17:37
Operator : CG/JU
Sample : N1340-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-6(1.5-2)

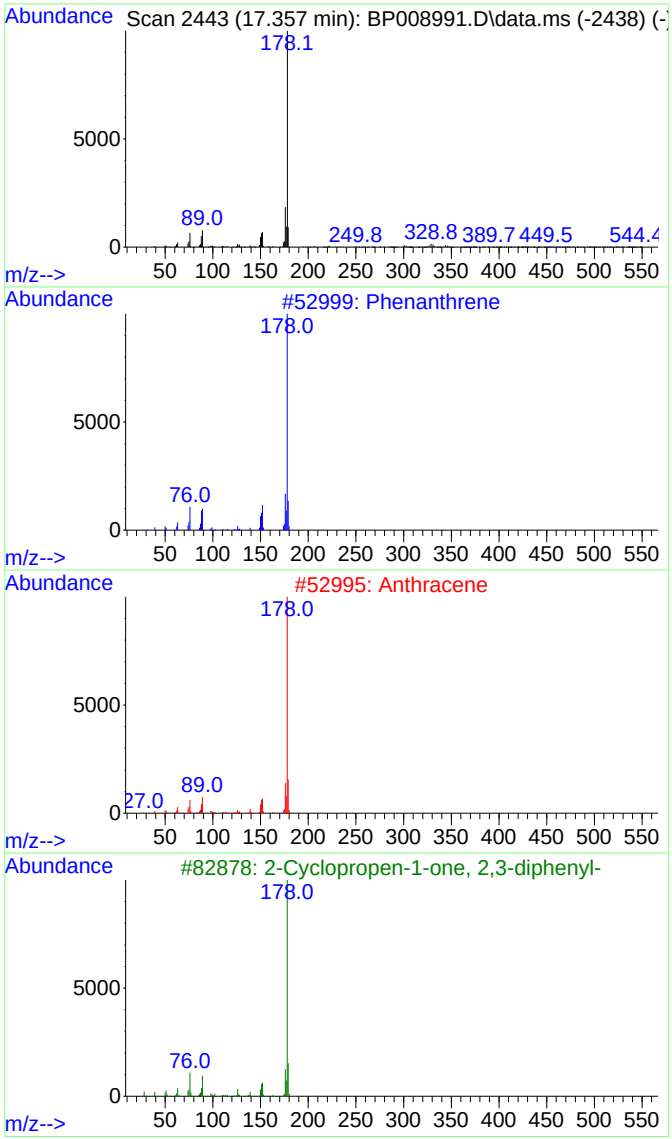
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP011422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

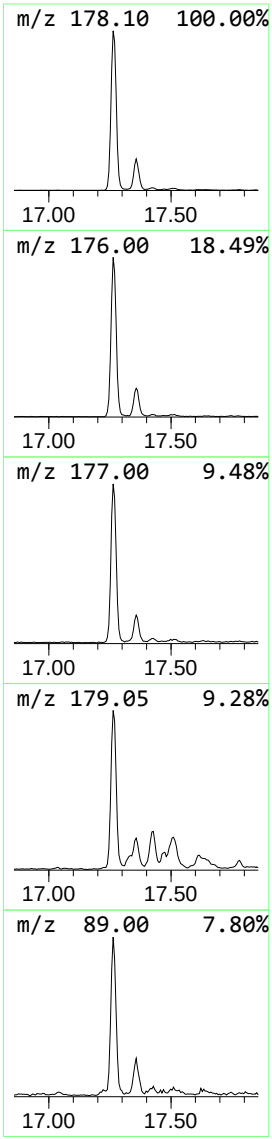
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Cyclopropen-1-one, 2,3-di... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.357	2.01 ng	277180	Phenanthrene-d10	17.222

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene	178	C14H10	000085-01-8	81
2	Anthracene	178	C14H10	000120-12-7	81
3	2-Cyclopropen-1-one, 2,3-diphenyl-	206	C15H10O	000886-38-4	80
4	4-Ethynyl-1,1'-biphenyl	178	C14H10	029079-00-3	74
5	4,9[1',2']-Benzeno-1H-benz[f]iso...	333	C21H19NO3	327078-94-4	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020122\
Data File : BP008991.D
Acq On : 01 Feb 2022 17:37
Operator : CG/JU
Sample : N1340-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-6(1.5-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP011422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

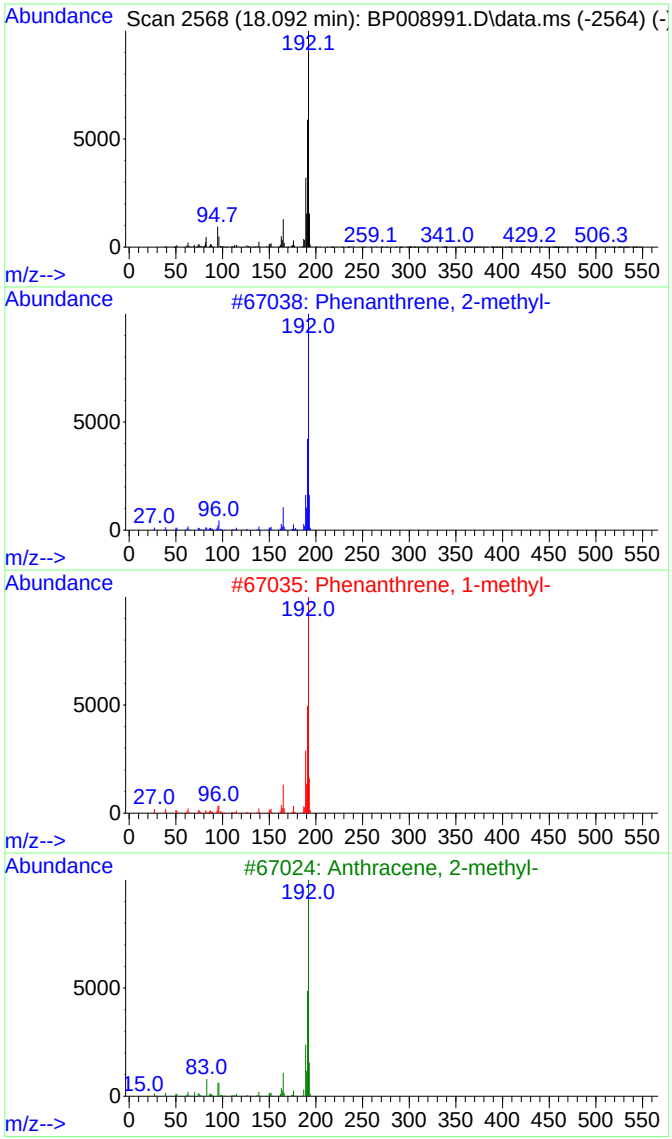
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

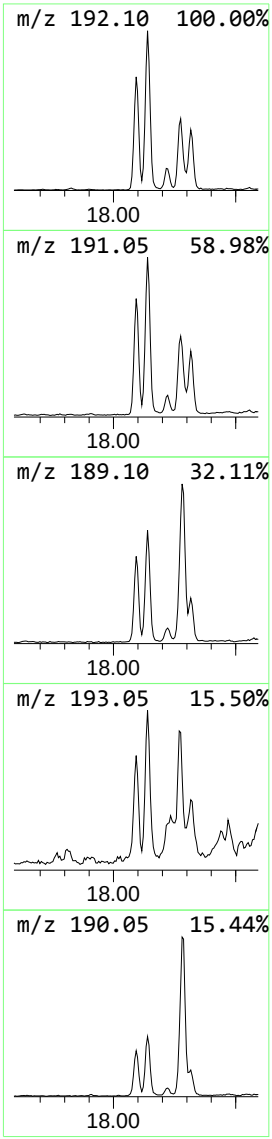
****

Peak Number 5 Phenanthrene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.092	2.16 ng	297942	Phenanthrene-d10	17.222

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
4	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	95
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020122\
Data File : BP008991.D
Acq On : 01 Feb 2022 17:37
Operator : CG/JU
Sample : N1340-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-6(1.5-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP011422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

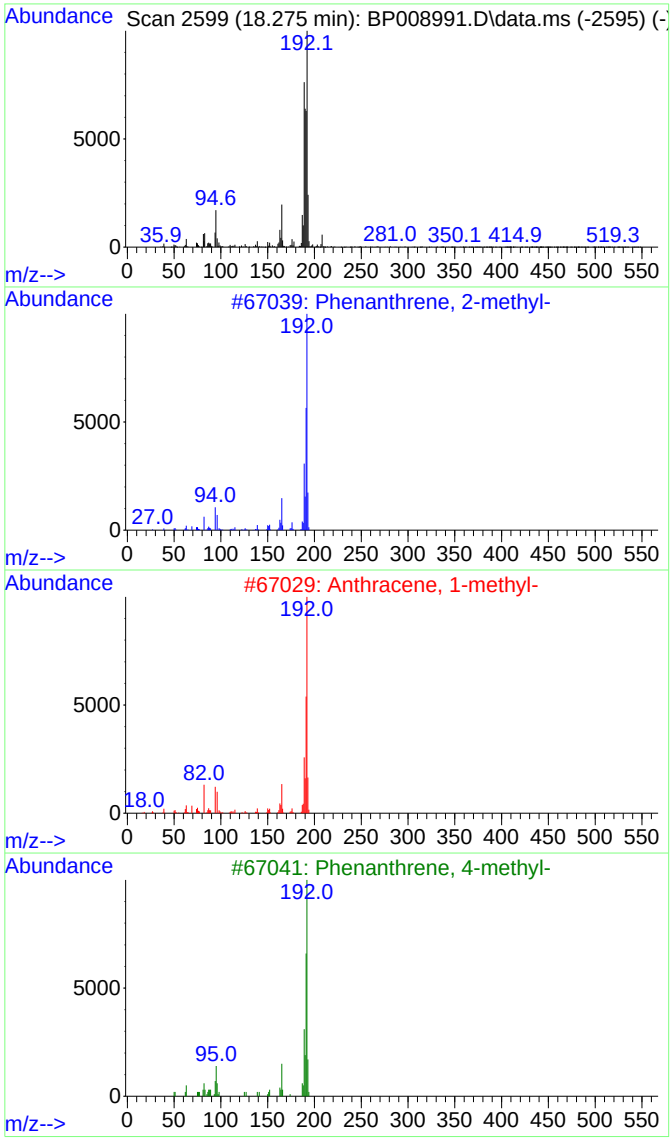
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

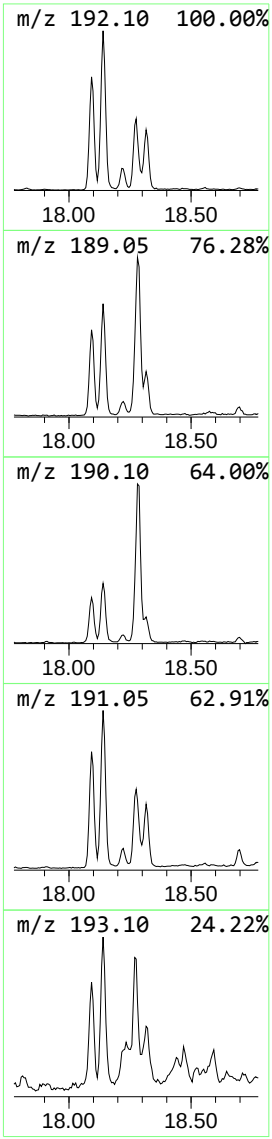
****

Peak Number 6 Anthracene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.275	2.78 ng	383838	Phenanthrene-d10	17.222

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	55
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	55
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	50
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	50
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020122\
Data File : BP008991.D
Acq On : 01 Feb 2022 17:37
Operator : CG/JU
Sample : N1340-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-6(1.5-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP011422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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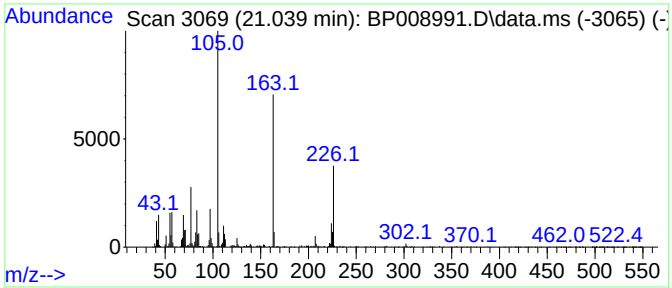
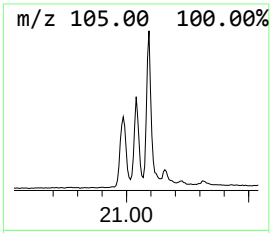
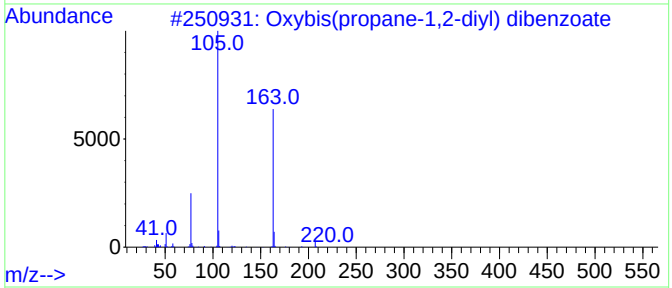
Peak Number 7 unknown21.039 Concentration Rank 2

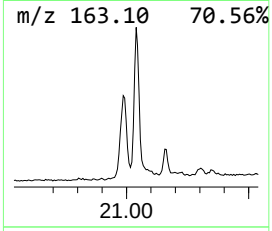
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.039	3.41 ng	721809	Chrysene-d12	21.316

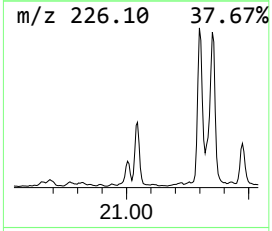
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	38
2	1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	37
3	Ethanone, 1-[2-(dimethylamino)ph...	163	C10H13NO	010336-55-7	37
4	Benzoic acid, (3-methylphenyl)me...	226	C15H14O2	1000368-97-4	27
5	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	25

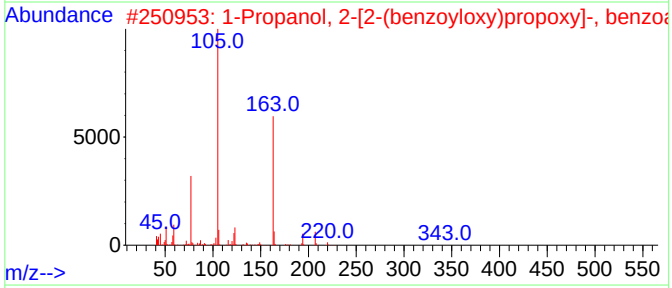


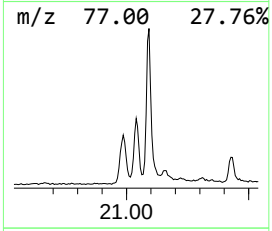


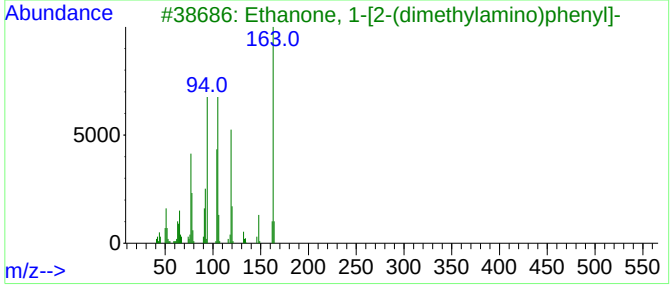


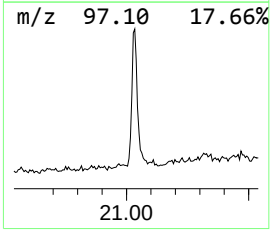












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020122\
Data File : BP008991.D
Acq On : 01 Feb 2022 17:37
Operator : CG/JU
Sample : N1340-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-6(1.5-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP011422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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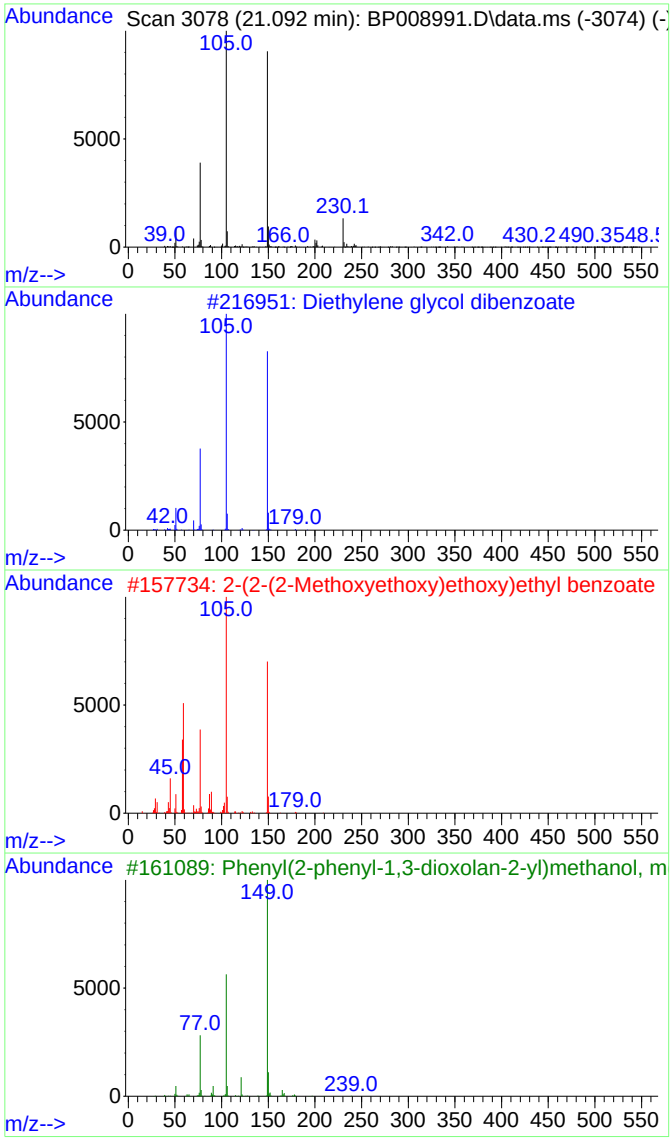
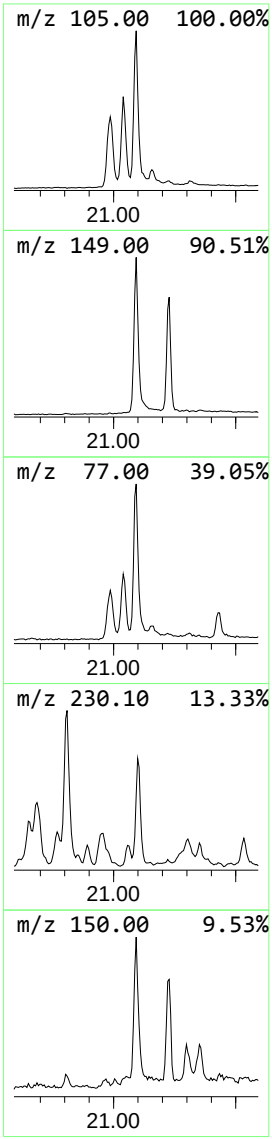
Peak Number 8 Diethylene glycol dibenzoate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.092	3.03 ng	641484	Chrysene-d12	21.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	80
2	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	72
3	Phenyl(2-phenyl-1,3-dioxolan-2-y...	270	C17H18O3	1000507-07-6	72
4	Phenyl(2-phenyl-1,3-dioxolan-2-y...	298	C18H18O4	006963-16-2	72
5	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020122\
Data File : BP008991.D
Acq On : 01 Feb 2022 17:37
Operator : CG/JU
Sample : N1340-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-6(1.5-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP011422.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...	3.034	6.4	ng	422480	1	7.828	1327710	20.0
2-Pentanone, 4-...	4.952	2.7	ng	179978	1	7.828	1327710	20.0
Benzocyclohepta...	12.293	2.2	ng	194987	2	10.622	1772450	20.0
2-Cyclopropen-1...	17.357	2.0	ng	277180	4	17.222	2760660	20.0
Phenanthrene, 2...	18.092	2.2	ng	297942	4	17.222	2760660	20.0
Anthracene, 1-m...	18.275	2.8	ng	383838	4	17.222	2760660	20.0
unknown21.039	21.039	3.4	ng	721809	5	21.316	4228210	20.0
Diethylene glyc...	21.092	3.0	ng	641484	5	21.316	4228210	20.0