LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101124\
Data File : BF139773.D
Acq On : 11 Oct 2024 14:20
Operator : RC/JU
Sample : P4364-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-2.0-2.5

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_F\Methods\8270-BF100124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139773.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	3	10	22	rVB	1730510	2838227	100.00%	12.234%
2	5.087	504	509	521	rVB	115349	172024	6.06%	0.742%
3	5.498	574	579	600	rBV	1358129	2040181	71.88%	8.794%
4	6.510	745	751	777	rBV	1275152	1946830	68.59%	8.392%
5	6.869	807	812	817	rBV	334808	424614	14.96%	1.830%
6	7.428	901	907	917	rBV	935369	1220005	42.98%	5.259%
7	7.681	945	950	954	rBV	38819	50310	1.77%	0.217%
8	7.728	954	958	972	rVB	33875	57096	2.01%	0.246%
9	8.145	1022	1029	1038	rBV2	365337	720536	25.39%	3.106%
10	8.363	1062	1066	1072	rBV	32777	43562	1.53%	0.188%
11	8.422	1072	1076	1085	rVB	25205	35374	1.25%	0.152%
12	9.222	1207	1212	1217	rBV	1415851	1738356	61.25%	7.493%
13	9.898	1319	1327	1332	rBV	327907	440823	15.53%	1.900%
14	10.316	1392	1398	1403	rVB2	26389	50644	1.78%	0.218%
15	10.616	1444	1449	1455	rVB	250435	317132	11.17%	1.367%
16	10.692	1456	1462	1469	rVV	767485	994058	35.02%	4.285%
17	10.751	1469	1472	1477	rVV	21239	38195	1.35%	0.165%
18	10.804	1477	1481	1489	rVB2	29476	52936	1.87%	0.228%
19	11.280	1559	1562	1568	rVB2	25412	38421	1.35%	0.166%
20	11.386	1575	1580	1583	rBV	339809	495161	17.45%	2.134%
21	11.463	1589	1593	1597	rBV	39526	46254	1.63%	0.199%
22	11.622	1616	1620	1625	rBV2	25600	42071	1.48%	0.181%
23	11.845	1653	1658	1661	rBV2	39536	75324	2.65%	0.325%
24	11.916	1663	1670	1672	rVV2	359138	524748	18.49%	2.262%
25	11.951	1672	1676	1681	rVV	1077522	1391066	49.01%	5.996%
26	12.004	1681	1685	1693	rVB2	60727	126430	4.45%	0.545%
27	12.439	1756	1759	1762	rBV	27645	38747	1.37%	0.167%
28	12.527	1771	1774	1779	rVB	28025	34930	1.23%	0.151%
29	12.604	1782	1787	1791	rBV	366549	484361	17.07%	2.088%
30	12.698	1799	1803	1810	rBV	81719	118790	4.19%	0.512%
31	12.833	1819	1826	1830	rBV	333362	510001	17.97%	2.198%
32	12.974	1844	1850	1857	rVB	1299596	1676403	59.07%	7.226%
33	13.051	1859	1863	1867	rBV3	32249	53979	1.90%	0.233%
34	13.263	1896	1899	1906	rVB3	37143	51531	1.82%	0.222%
35	13.645	1960	1964	1967	rBV	161952	228838	8.06%	0.986%
36	13.680	1967	1970	1975	rVB3	128931	190461	6.71%	0.821%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101124\
Data File : BF139773.D
Acq On : 11 Oct 2024 14:20
Operator : RC/JU
Sample : P4364-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-2.0-2.5

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_F\Methods\8270-BF100124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.786	1984	1988	1994	rBV4	40774	97102	3.42%	0.419%
38	13.880	2000	2004	2008	rBV4	88939	149820	5.28%	0.646%
39	14.010	2021	2026	2033	rBV3	1038989	2196674	77.40%	9.469%
40	14.415	2091	2095	2099	rBV2	114777	143242	5.05%	0.617%
41	14.621	2126	2130	2136	rVB	119715	181554	6.40%	0.783%
42	15.074	2203	2207	2215	rVB	162092	323020	11.38%	1.392%
43	15.380	2256	2259	2265	rVB	90120	137113	4.83%	0.591%
44	15.445	2266	2270	2275	rVV	122513	192871	6.80%	0.831%
45	15.509	2276	2281	2298	rVB2	230529	468910	16.52%	2.021%

Sum of corrected areas: 23198725

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101124\
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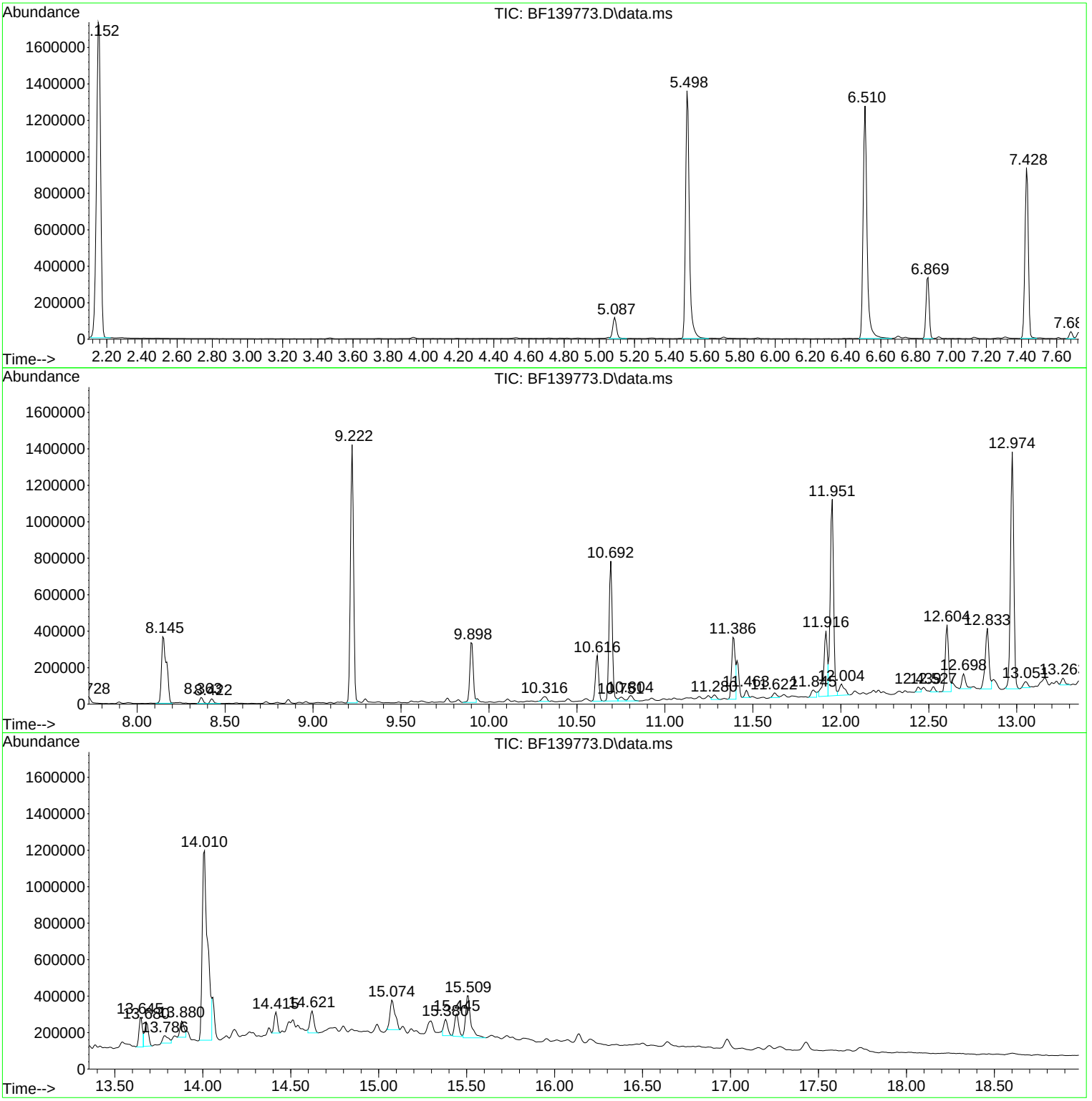
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-2.0-2.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.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_F\Data\BF101124\
Data File : BF139773.D
Acq On : 11 Oct 2024 14:20
Operator : RC/JU
Sample : P4364-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-2.0-2.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

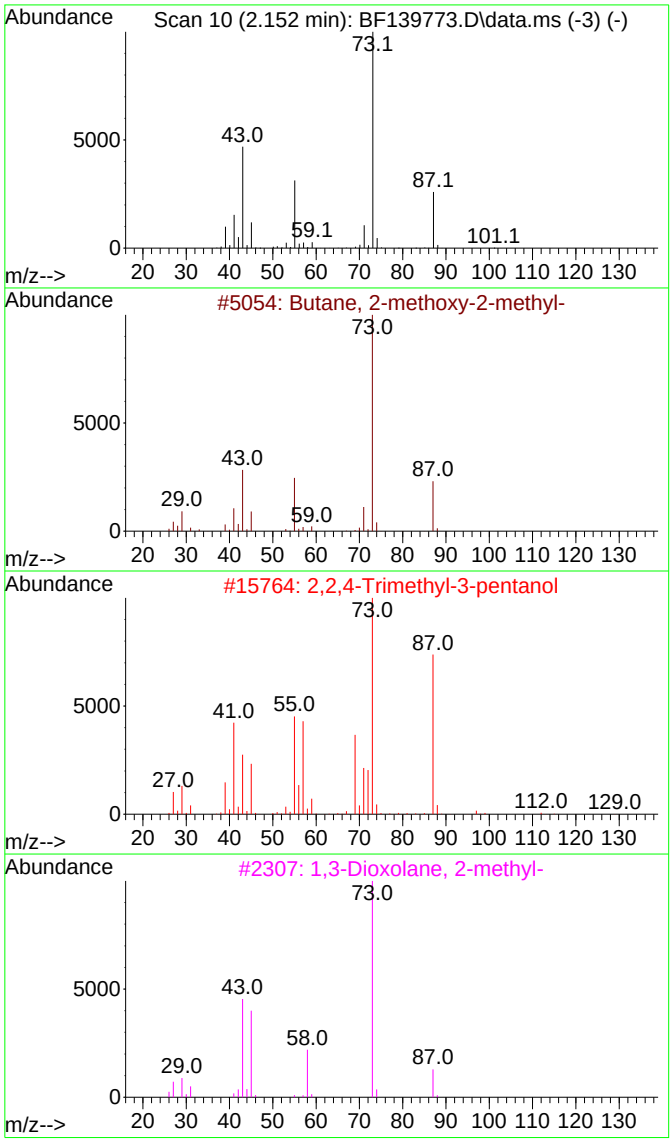
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

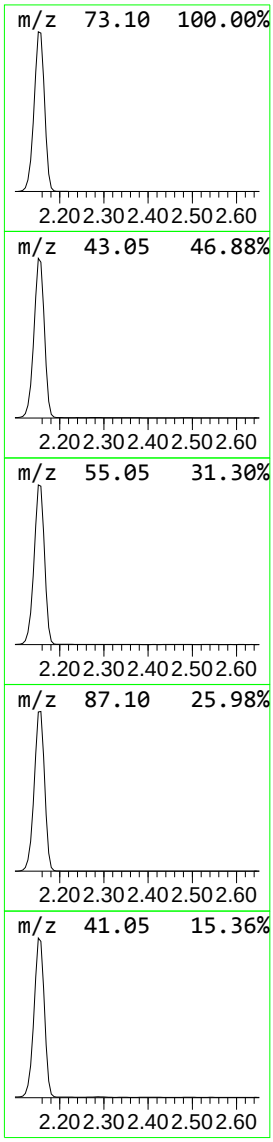
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	133.69 ng	2838230	1,4-Dichlorobenzene-d4	6.869

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	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101124\
Data File : BF139773.D
Acq On : 11 Oct 2024 14:20
Operator : RC/JU
Sample : P4364-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-2.0-2.5

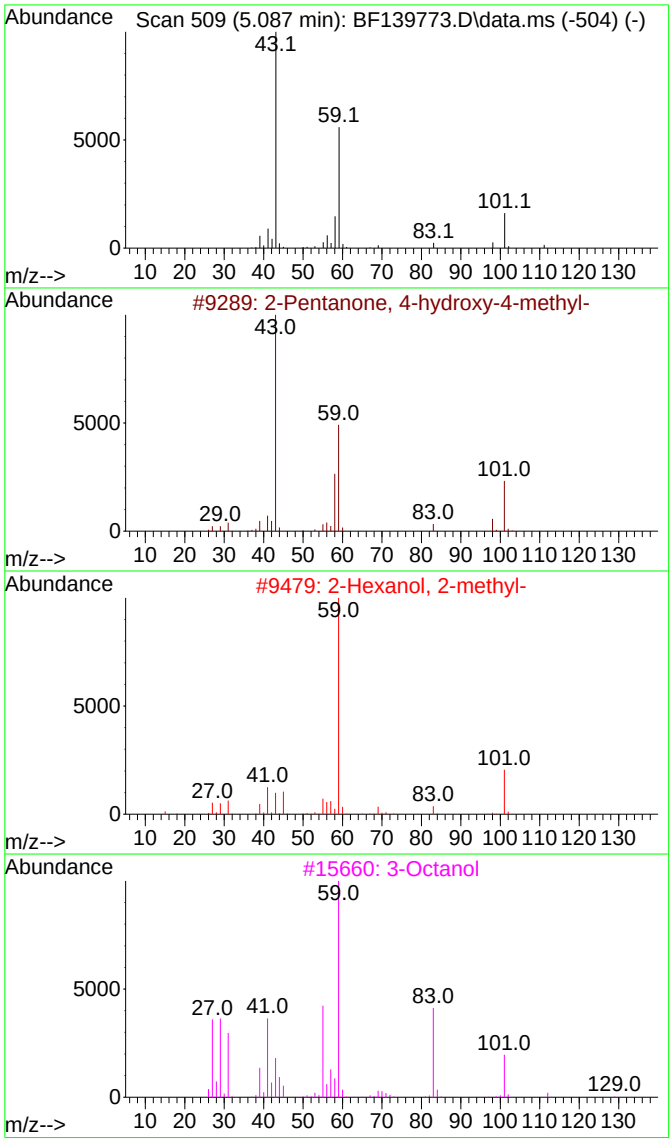
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

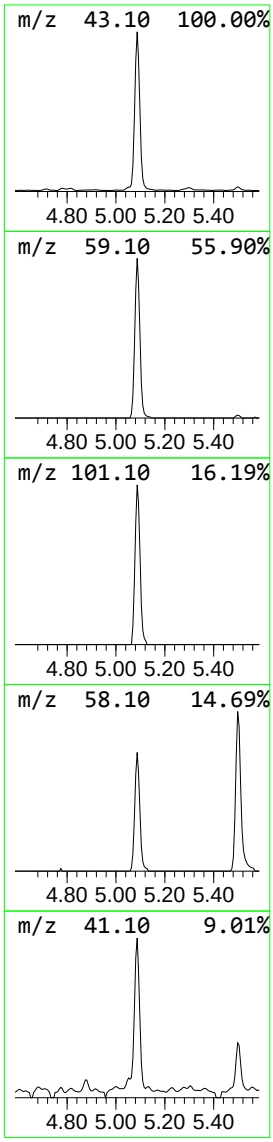
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	8.10 ng	172024	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	37
3	3-Octanol	130	C8H18O	000589-98-0	33
4	3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101124\
Data File : BF139773.D
Acq On : 11 Oct 2024 14:20
Operator : RC/JU
Sample : P4364-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-2.0-2.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

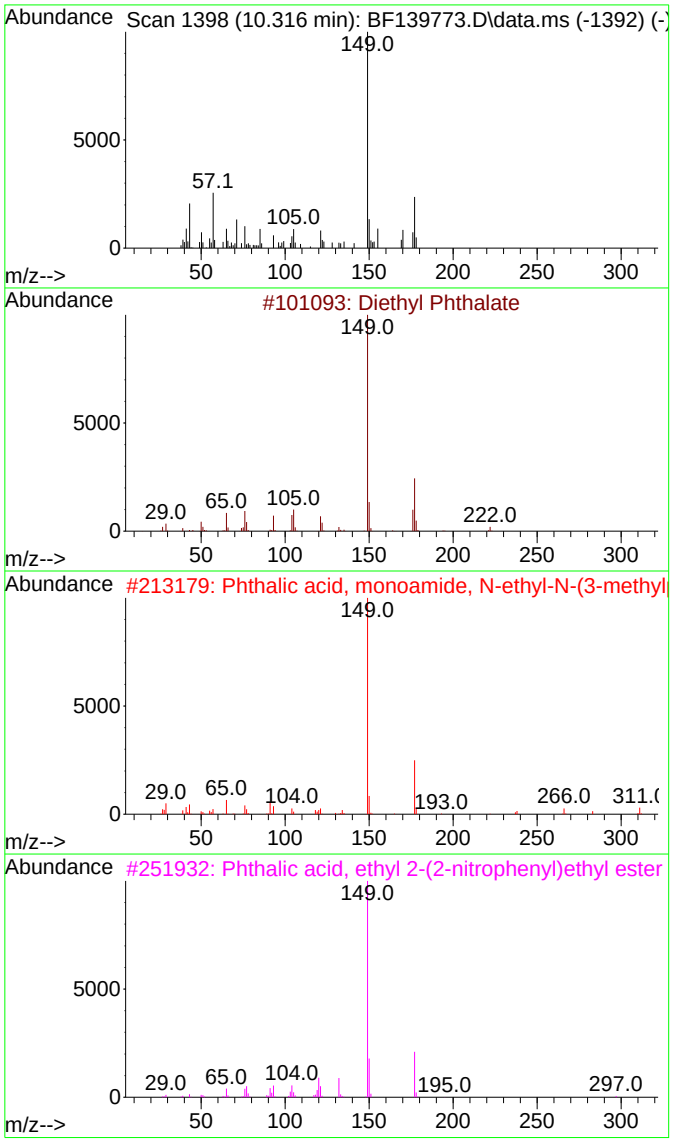
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

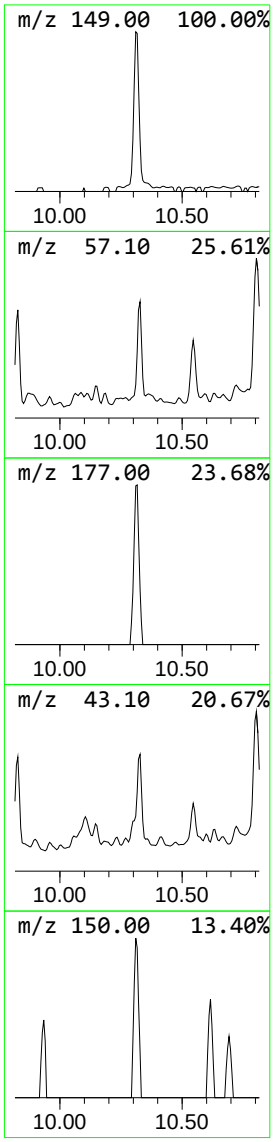
****

Peak Number 3 Phthalic acid, monoamide, N... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.316	2.30 ng	50644	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyl Phthalate	222	C12H14O4	000084-66-2	80
2	Phthalic acid, monoamide, N-ethy...	311	C19H21NO3	1000309-85-4	64
3	Phthalic acid, ethyl 2-(2-nitrop...	343	C18H17NO6	1000377-99-1	59
4	2-Acetylbenzoic acid	164	C9H8O3	000577-56-0	50
5	Benzoic acid, 2-(1-oxopropyl)-	178	C10H10O3	002360-45-4	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101124\
Data File : BF139773.D
Acq On : 11 Oct 2024 14:20
Operator : RC/JU
Sample : P4364-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-2.0-2.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

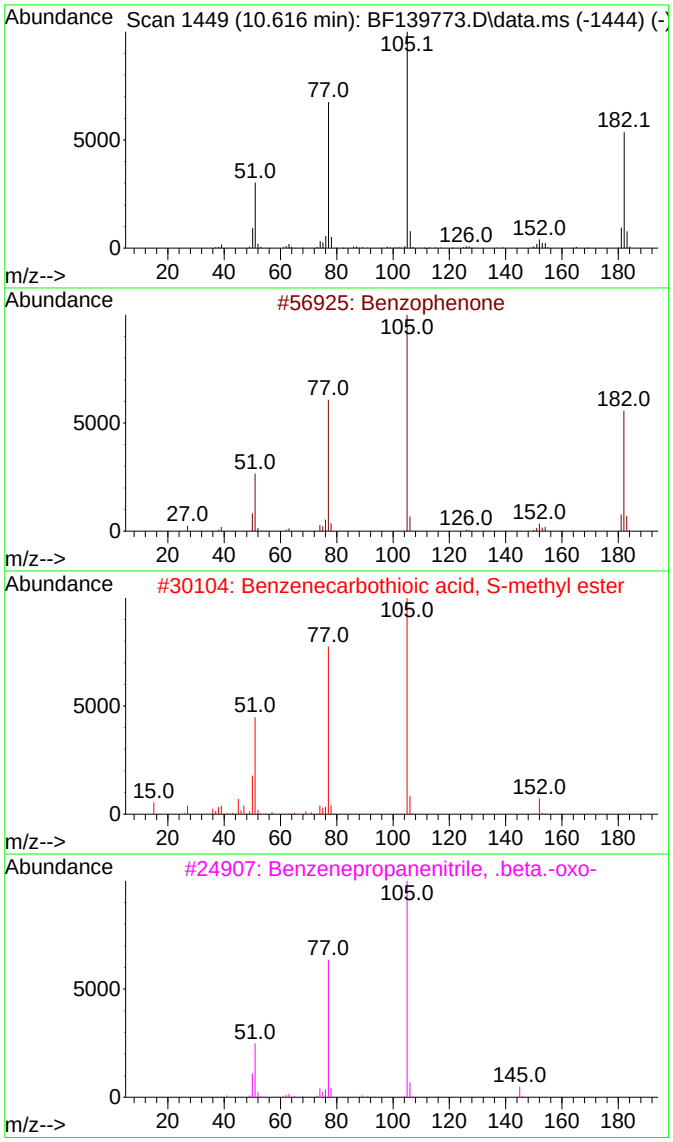
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

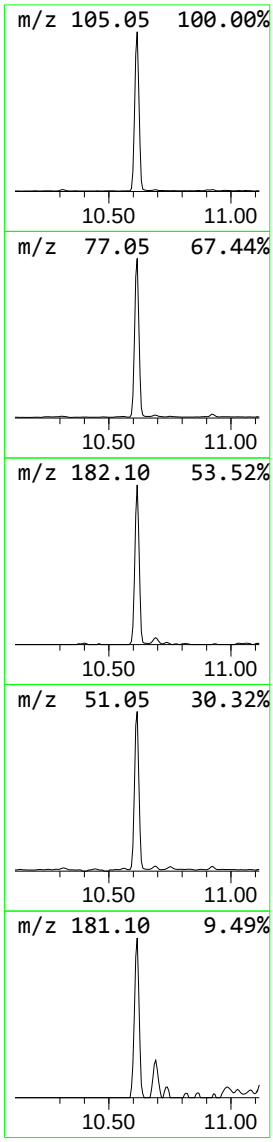
****

Peak Number 4 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.616	14.39 ng	317132	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
3	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
4	1-Butanone, 1-phenyl-	148	C10H12O	000495-40-9	47
5	2,5-Pyrrolidinedione, 1-(benzoyl...	219	C11H9NO4	023405-15-4	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101124\
Data File : BF139773.D
Acq On : 11 Oct 2024 14:20
Operator : RC/JU
Sample : P4364-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-2.0-2.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

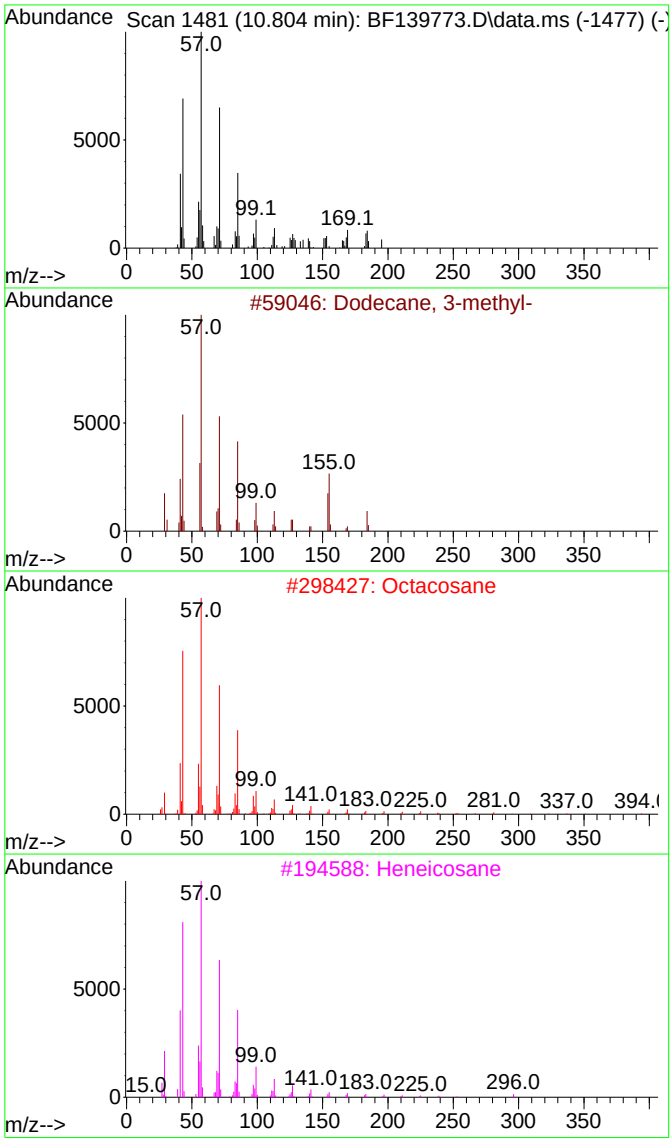
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

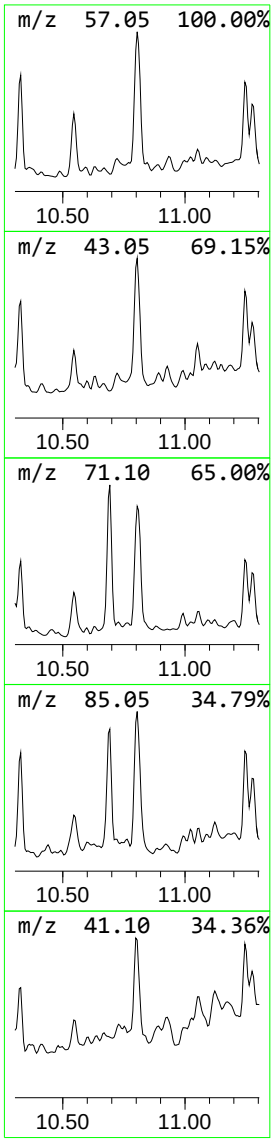
****

Peak Number 5 Dodecane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.804	2.14 ng	52936	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 3-methyl-	184	C13H28	017312-57-1	81
2	Octacosane	394	C28H58	000630-02-4	74
3	Heneicosane	296	C21H44	000629-94-7	74
4	Tridecane	184	C13H28	000629-50-5	74
5	Hexacosane	366	C26H54	000630-01-3	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101124\
Data File : BF139773.D
Acq On : 11 Oct 2024 14:20
Operator : RC/JU
Sample : P4364-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-2.0-2.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

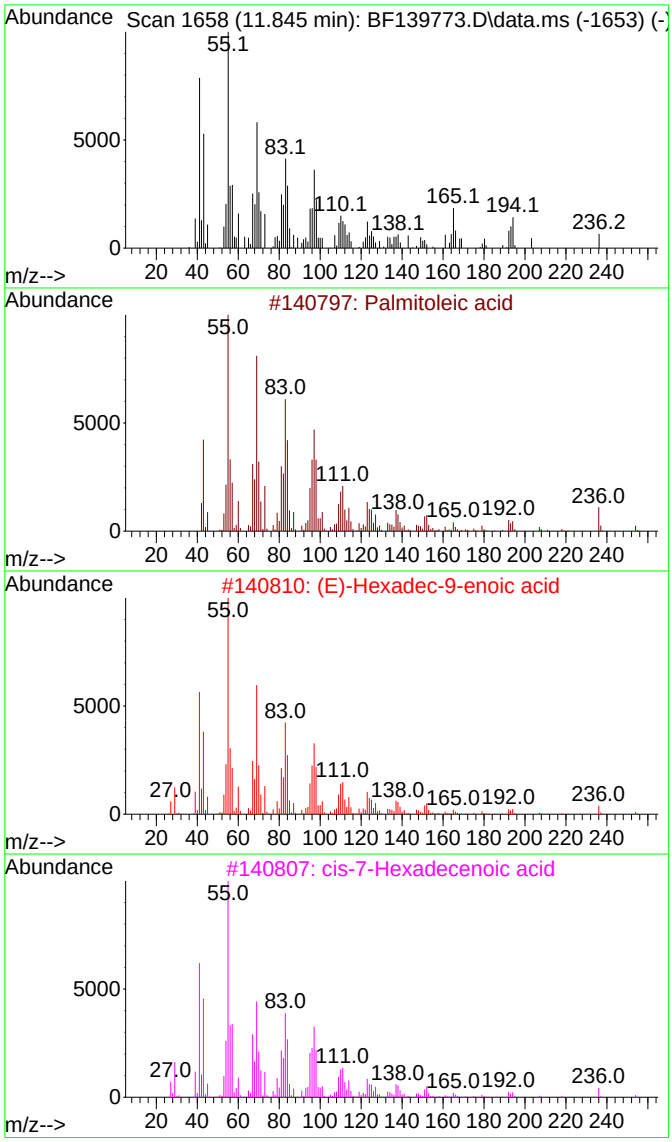
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

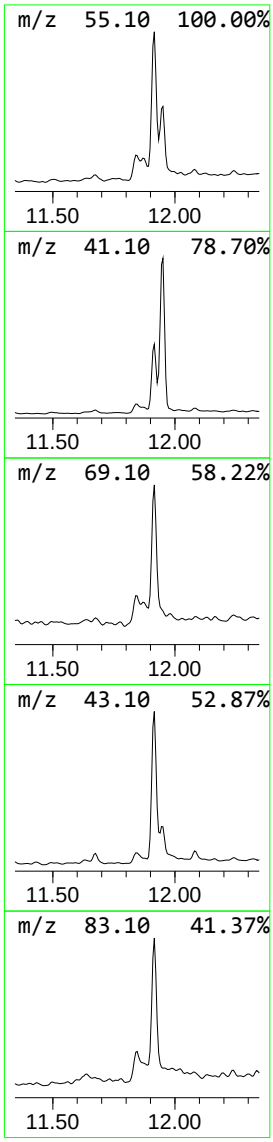
****

Peak Number 6 Palmitoleic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.845	3.04 ng	75324	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Palmitoleic acid	254	C16H30O2	000373-49-9	81
2	(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	76
3	cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	70
4	Z-7-Tetradecenoic acid	226	C14H26O2	1000130-98-4	64
5	Myristoleic acid	226	C14H26O2	000544-64-9	58





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Sample : P4364-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-2.0-2.5

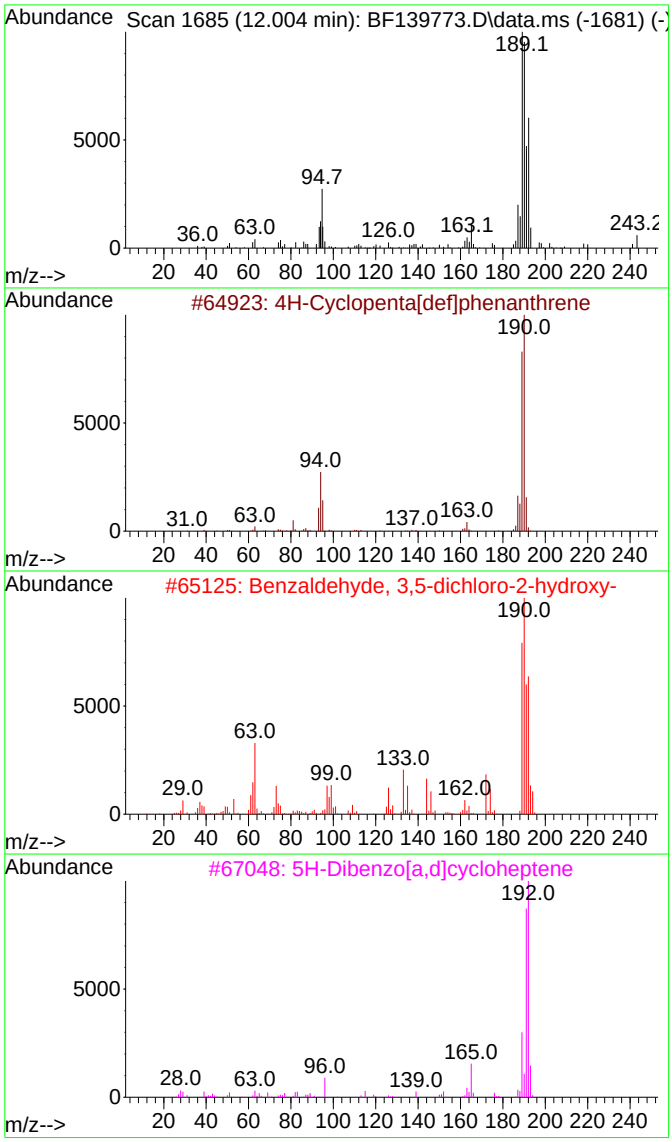
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

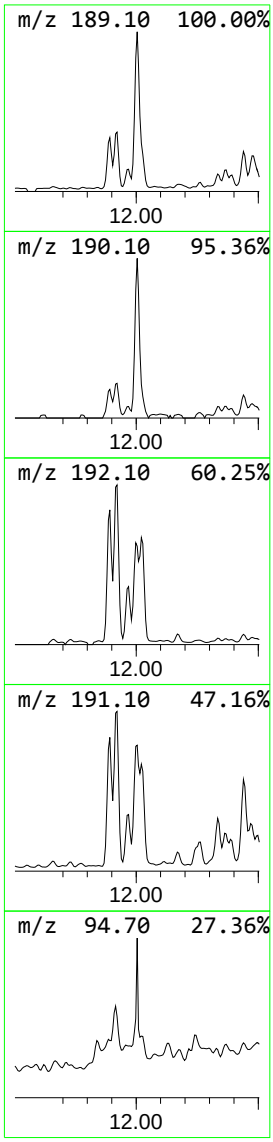
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.004	5.11 ng	126430	Phenanthrene-d10	11.386

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	47
3	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	38
4	Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	38
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101124\
Data File : BF139773.D
Acq On : 11 Oct 2024 14:20
Operator : RC/JU
Sample : P4364-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-2.0-2.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

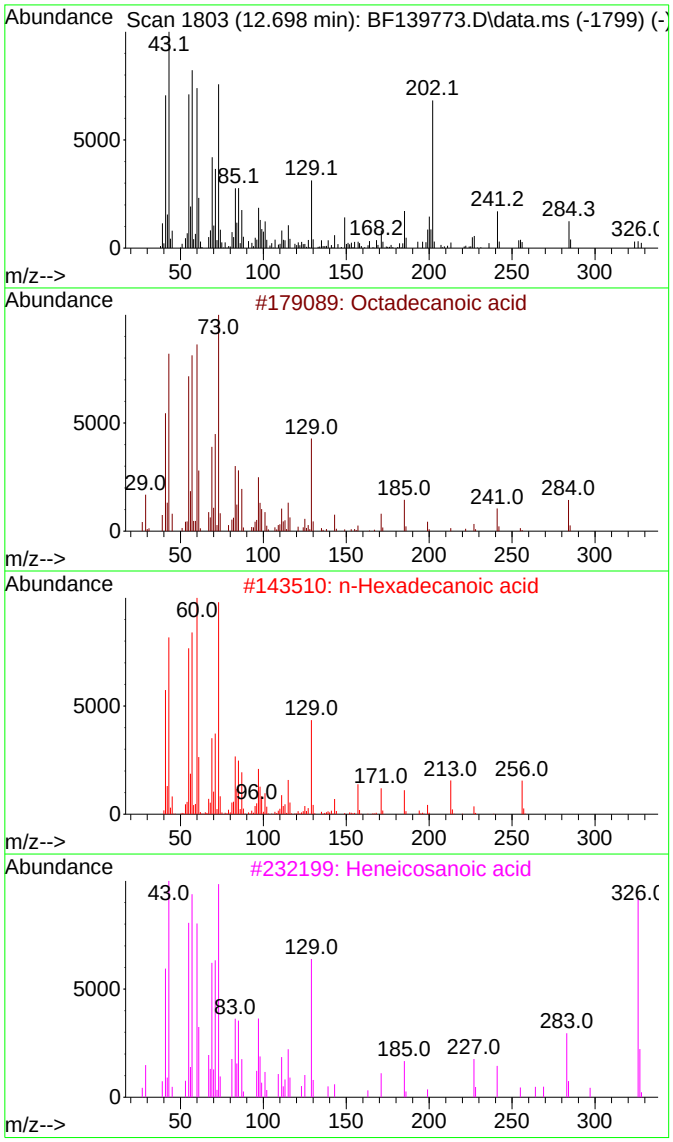
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

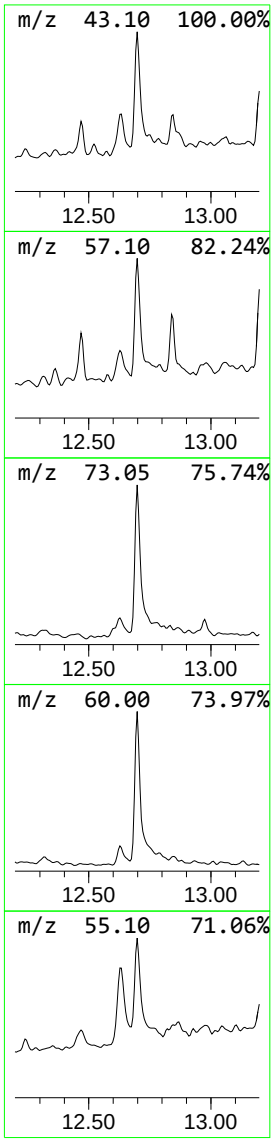
****

Peak Number 8 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.698	4.80 ng	118790	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	Heneicosanoic acid	326	C21H42O2	002363-71-5	86
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	68
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





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Operator : RC/JU
Sample : P4364-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-04-2.0-2.5

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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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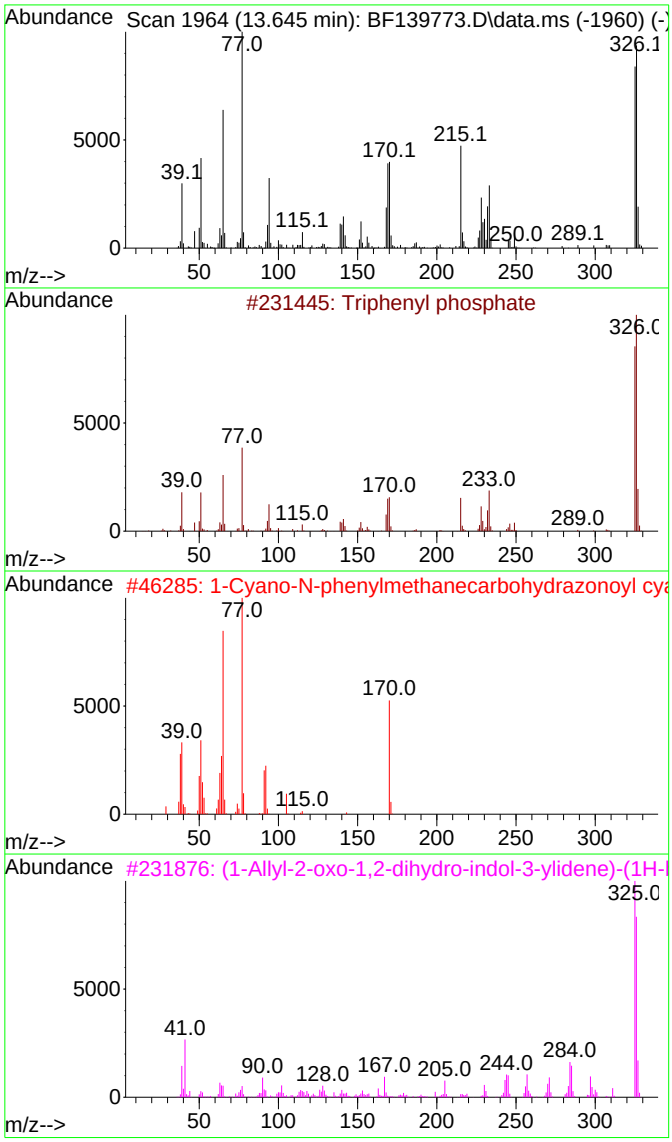
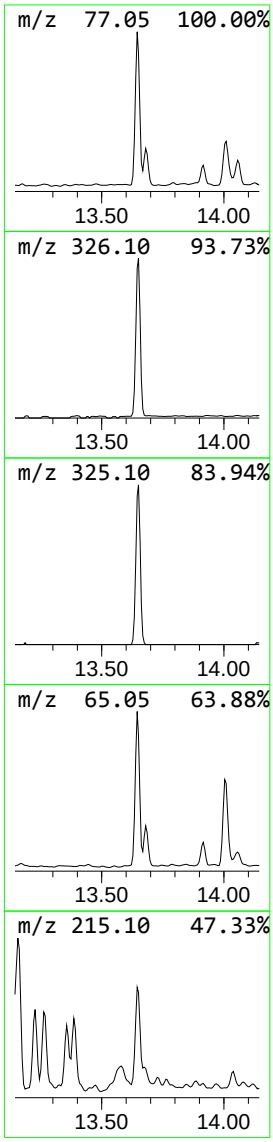
Peak Number 9 Triphenyl phosphate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.645	2.08 ng	228838	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenyl phosphate	326	C18H15O4P	000115-86-6	96
2	1-Cyano-N-phenylmethanecarbohydr...	170	C9H6N4	000306-18-3	38
3	(1-Allyl-2-oxo-1,2-dihydro-indol...	326	C20H14N4O	1000296-28-1	14
4	2-Methyl-3,8-diphenyl-3H-imidazo...	325	C21H15N3O	089174-96-9	14
5	Benzene, (ethylsulfonyl)-	170	C8H10O2S	000599-70-2	11





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101124\
Data File : BF139773.D
Acq On : 11 Oct 2024 14:20
Operator : RC/JU
Sample : P4364-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-2.0-2.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.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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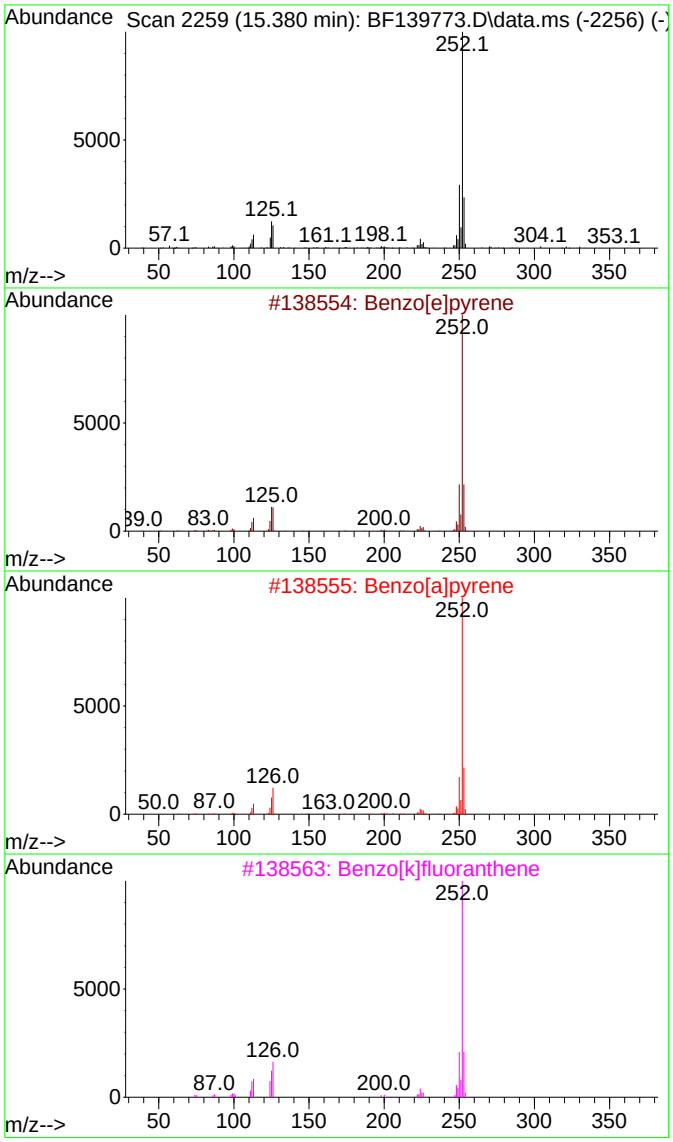
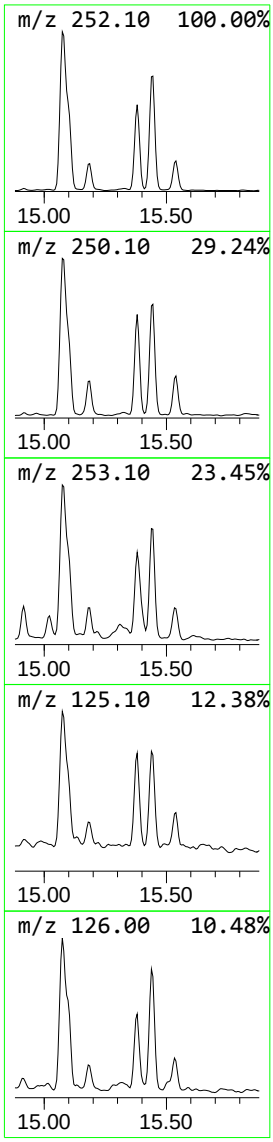
Peak Number 10 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.380	5.85 ng	137113	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[a]pyrene	252	C20H12	000050-32-8	96
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
4	Perylene	252	C20H12	000198-55-0	95
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	95





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101124\
Data File : BF139773.D
Acq On : 11 Oct 2024 14:20
Operator : RC/JU
Sample : P4364-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-2.0-2.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.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...	2.152	133.7	ng	2838230	1	6.869	424614	20.0
2-Pentanone, 4-...	5.087	8.1	ng	172024	1	6.869	424614	20.0
Phthalic acid, ...	10.316	2.3	ng	50644	3	9.904	440823	20.0
Benzophenone	10.616	14.4	ng	317132	3	9.904	440823	20.0
Dodecane, 3-met...	10.804	2.1	ng	52936	4	11.386	495161	20.0
Palmitoleic acid	11.845	3.0	ng	75324	4	11.386	495161	20.0
4H-Cyclopenta[d...	12.004	5.1	ng	126430	4	11.386	495161	20.0
Octadecanoic acid	12.698	4.8	ng	118790	4	11.386	495161	20.0
Triphenyl phosp...	13.645	2.1	ng	228838	5	14.033	2196670	20.0
Benzo[e]pyrene	15.380	5.8	ng	137113	6	15.504	468910	20.0