LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101124\
Data File : BF139769.D
Acq On : 11 Oct 2024 12:25
Operator : RC/JU
Sample : P4364-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-08-0.167-0.667

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: BF139769.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	9	24	rVB	1464972	2295117	100.00%	13.311%
2	5.081	503	508	518	rVB	91039	132974	5.79%	0.771%
3	5.487	571	577	594	rVB	1270024	1665772	72.58%	9.661%
4	6.498	743	749	765	rBV	1233226	1627999	70.93%	9.442%
5	6.863	806	811	817	rBV	367055	465752	20.29%	2.701%
6	7.428	901	907	912	rBV	823344	1039353	45.29%	6.028%
7	7.681	945	950	954	rBV	36103	47682	2.08%	0.277%
8	7.722	954	957	962	rVB	20828	28114	1.22%	0.163%
9	8.145	1021	1029	1038	rBV	426832	558100	24.32%	3.237%
10	8.363	1062	1066	1072	rBV	29025	37606	1.64%	0.218%
11	8.422	1072	1076	1082	rVB	22944	27941	1.22%	0.162%
12	9.222	1207	1212	1217	rBV	1338774	1627461	70.91%	9.439%
13	9.298	1221	1225	1231	rVB2	19799	26536	1.16%	0.154%
14	9.898	1320	1327	1341	rVB	376363	493519	21.50%	2.862%
15	10.316	1392	1398	1403	rBV2	28677	54706	2.38%	0.317%
16	10.616	1443	1449	1456	rBV	226772	295034	12.85%	1.711%
17	10.692	1456	1462	1473	rVV	575896	769506	33.53%	4.463%
18	10.804	1476	1481	1489	rVB2	26473	48030	2.09%	0.279%
19	11.245	1552	1556	1559	rBV2	22848	29036	1.27%	0.168%
20	11.386	1575	1580	1589	rBV2	359985	547747	23.87%	3.177%
21	11.463	1589	1593	1596	rVB	18127	23244	1.01%	0.135%
22	11.675	1625	1629	1634	rVB2	16526	23885	1.04%	0.139%
23	11.910	1662	1669	1681	rBV3	189892	372170	16.22%	2.159%
24	11.998	1681	1684	1692	rVV	28046	60539	2.64%	0.351%
25	12.080	1694	1698	1703	rVV2	19676	29003	1.26%	0.168%
26	12.469	1762	1764	1771	rVB3	20225	25690	1.12%	0.149%
27	12.604	1782	1787	1791	rBV	210319	270375	11.78%	1.568%
28	12.698	1799	1803	1808	rBV	41002	65369	2.85%	0.379%
29	12.833	1820	1826	1831	rVB	209154	303367	13.22%	1.760%
30	12.974	1844	1850	1857	rVB	1133379	1463598	63.77%	8.489%
31	13.045	1859	1862	1870	rBV3	18636	37072	1.62%	0.215%
32	13.198	1885	1888	1891	rBV	26164	34151	1.49%	0.198%
33	13.263	1896	1899	1903	rVB2	26316	32444	1.41%	0.188%
34	13.669	1965	1968	1973	rVB	35083	47123	2.05%	0.273%
35	13.874	2000	2003	2013	rVB3	80141	151779	6.61%	0.880%
36	14.027	2023	2029	2041	rVB2	476275	924235	40.27%	5.360%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101124\
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Misc :
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Instrument :
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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	14.492	2105	2108	2113	rBV4	42523	57571	2.51%	0.334%
38	14.786	2153	2158	2165	rBV3	196333	311171	13.56%	1.805%
39	15.074	2202	2207	2214	rBV	165668	365063	15.91%	2.117%
40	15.374	2255	2258	2264	rVB	79966	123674	5.39%	0.717%
41	15.439	2265	2269	2275	rVB	110880	167591	7.30%	0.972%
42	15.504	2275	2280	2292	rBV2	241303	436232	19.01%	2.530%
43	16.980	2527	2531	2539	rVB2	52595	98302	4.28%	0.570%

Sum of corrected areas: 17241633

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101124\
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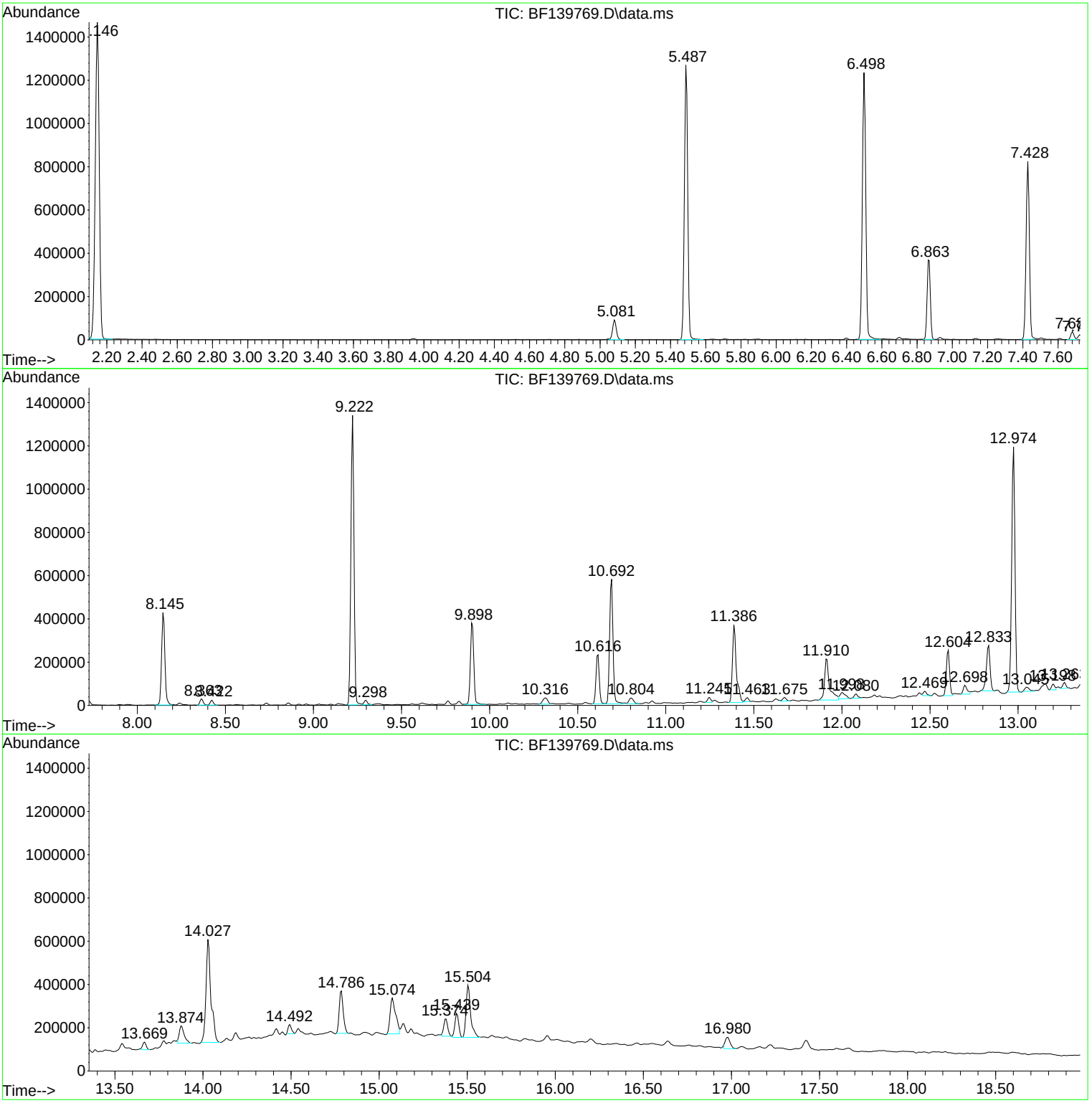
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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

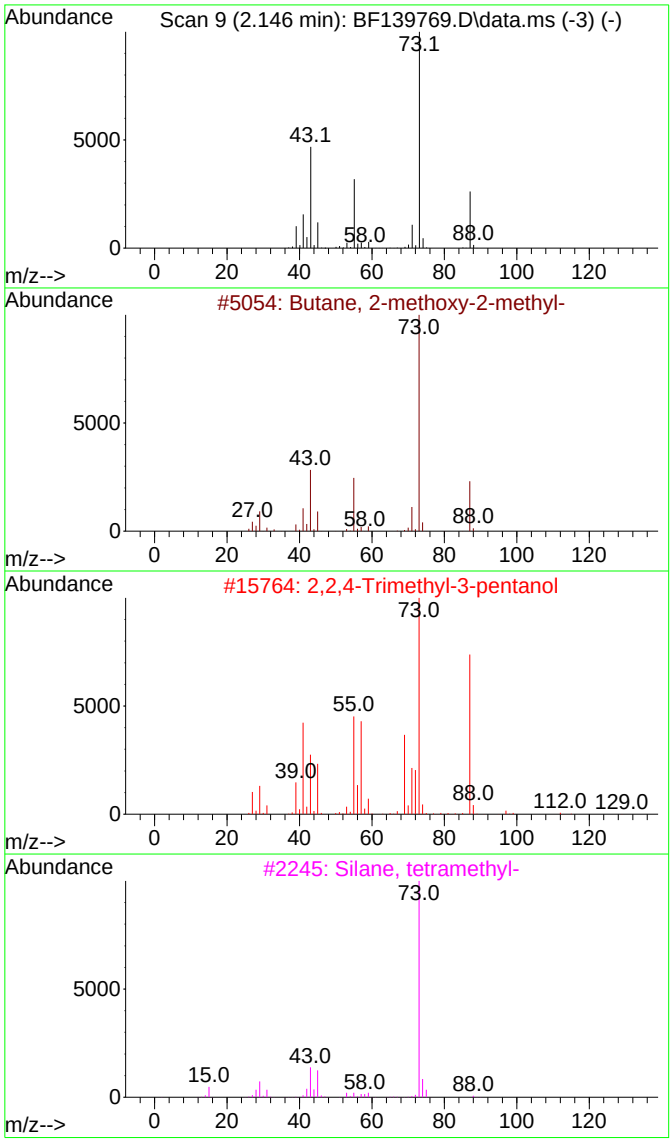
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

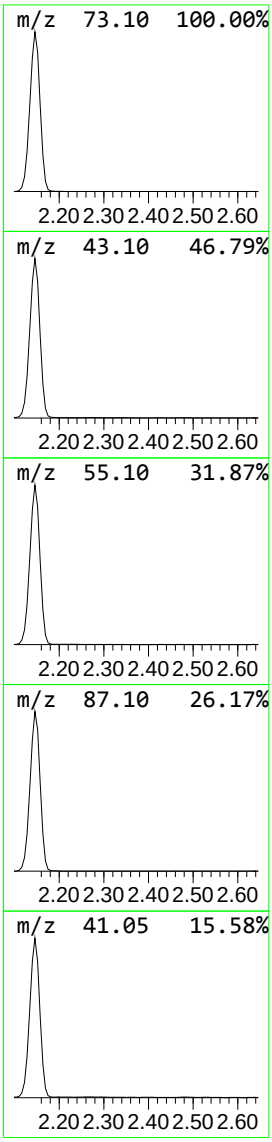
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	98.56 ng	2295120	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	39
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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Sample : P4364-16
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Instrument :
BNA_F
ClientSampleId :
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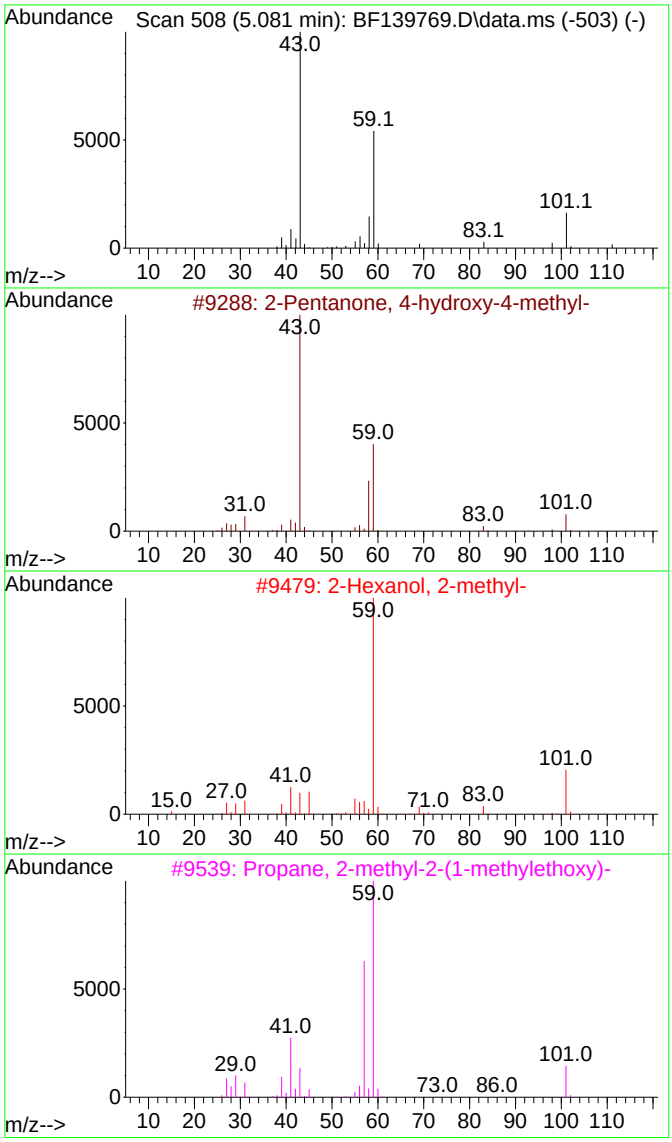
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

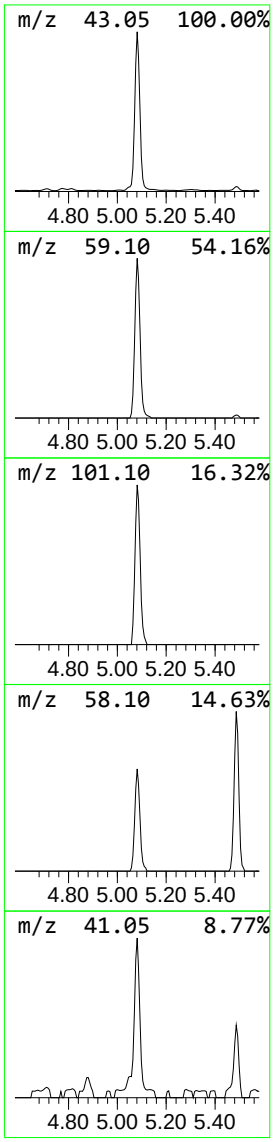
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	5.71 ng	132974	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	50
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	37
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	3-Octanol	130	C8H18O	000589-98-0	33





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Sample : P4364-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

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

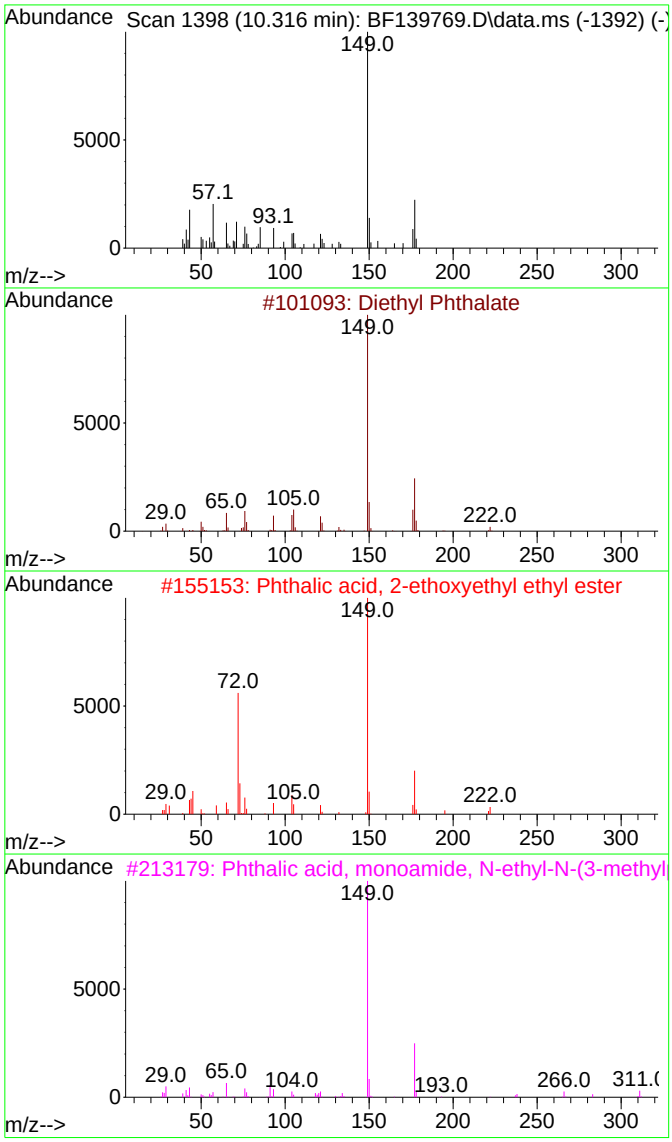
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

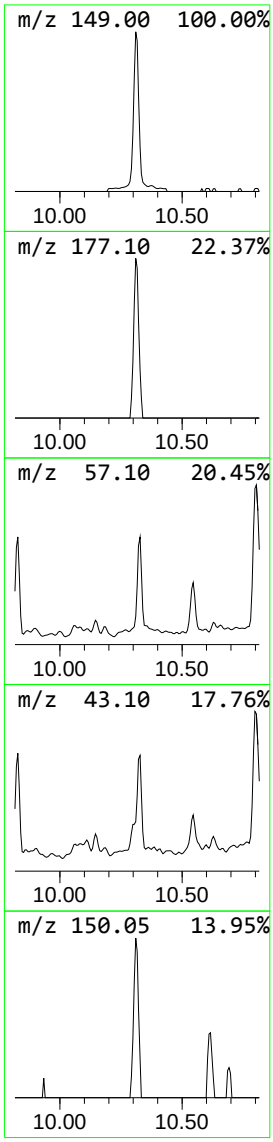
****

Peak Number 3 Phthalic acid, 2-ethoxyethy... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.316	2.22 ng	54706	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyl Phthalate	222	C12H14O4	000084-66-2	87
2	Phthalic acid, 2-ethoxyethyl eth...	266	C14H18O5	1000322-86-9	78
3	Phthalic acid, monoamide, N-ethy...	311	C19H21NO3	1000309-85-4	72
4	Phthalic acid, ethyl 2-(2-nitrop...	343	C18H17NO6	1000377-99-1	59
5	1,2-Benzenedicarboxylic acid, mo...	222	C12H14O4	000131-70-4	58





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Operator : RC/JU
Sample : P4364-16
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ALS Vial : 8 Sample Multiplier: 1

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

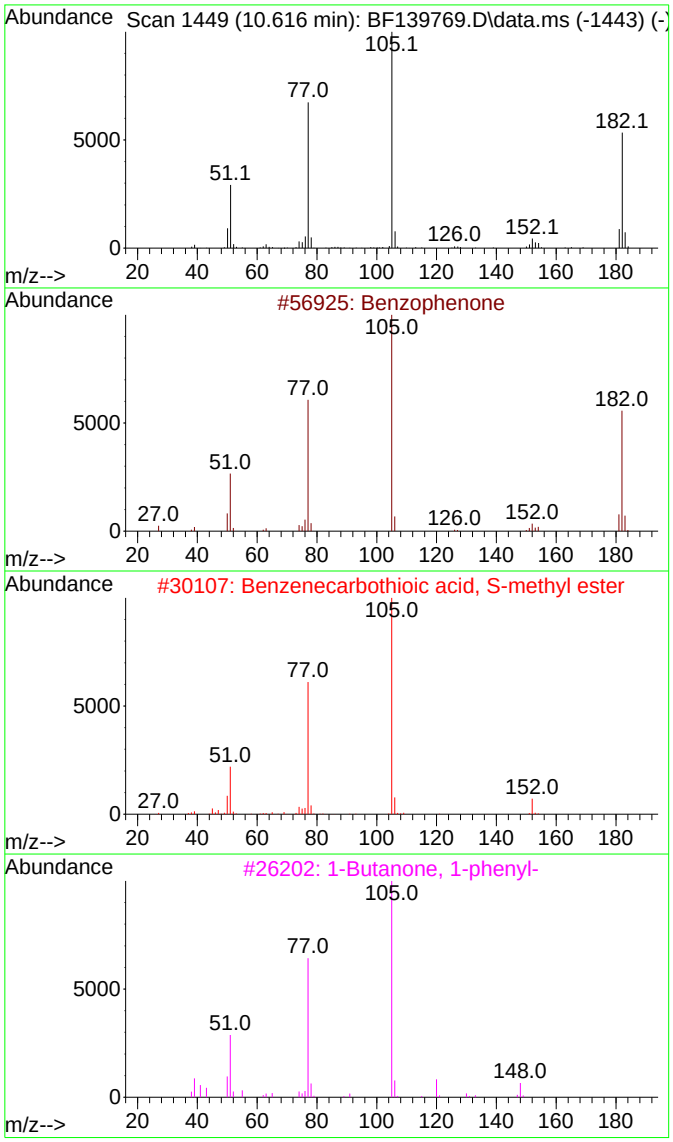
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

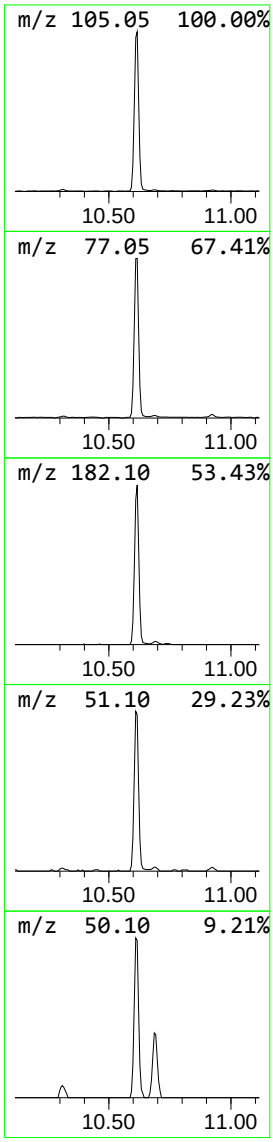
****

Peak Number 4 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.616	11.96 ng	295034	Acenaphthene-d10	9.898

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	58
3	1-Butanone, 1-phenyl-	148	C10H12O	000495-40-9	50
4	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	50
5	Methyl 2-benzoyl-4-cyanobutanoate	231	C13H13NO3	1010486-83-8	50





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Sample : P4364-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

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

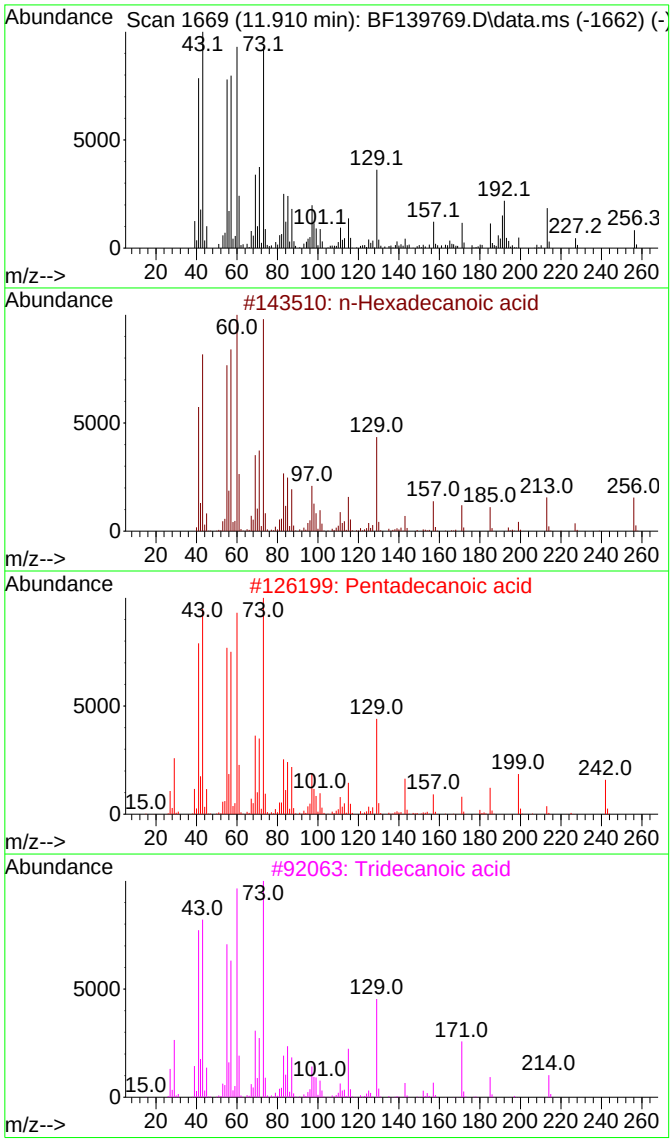
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

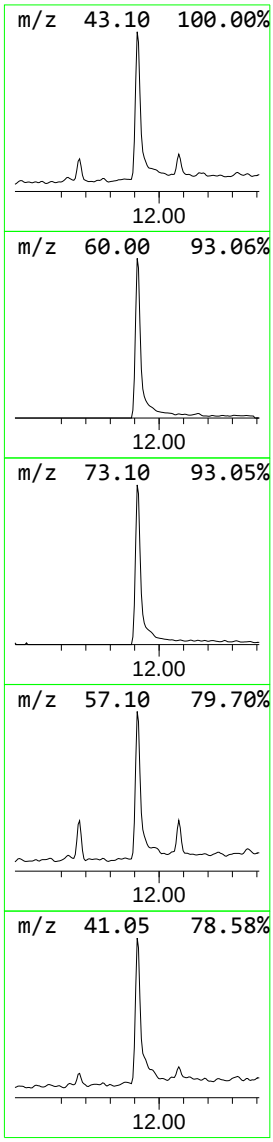
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	13.59 ng	372170	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Undecanoic acid	186	C11H22O2	000112-37-8	58





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ALS Vial : 8 Sample Multiplier: 1

Instrument :
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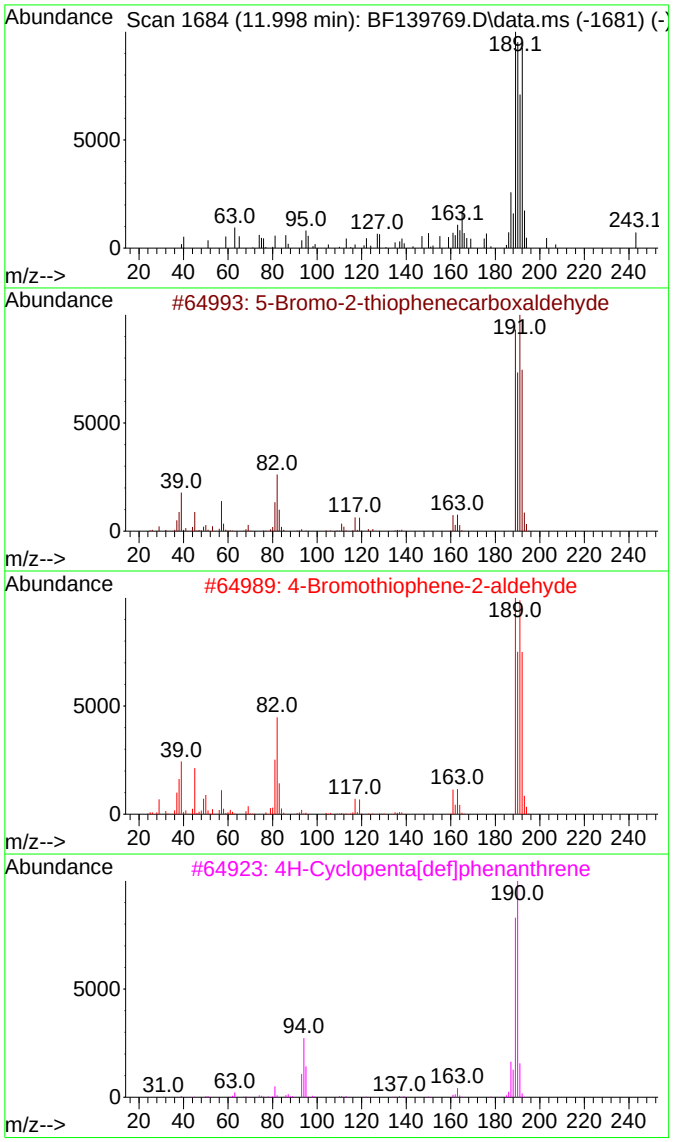
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

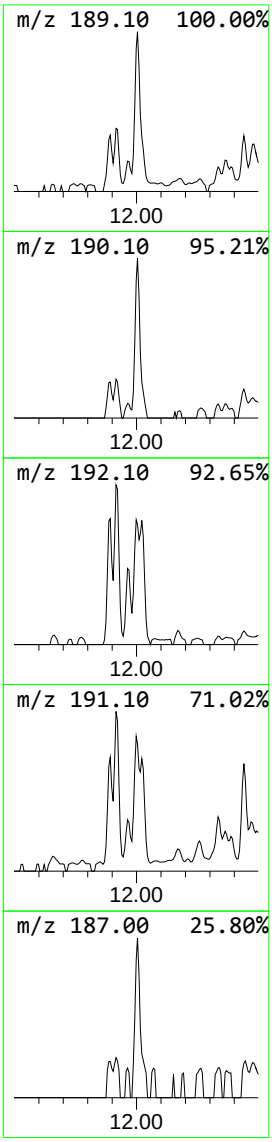
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 5-Bromo-2-thiophenecarboxal... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.998	2.21 ng	60539	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Bromo-2-thiophenecarboxaldehyde	190	C5H3BrOS	004701-17-1	64
2	4-Bromothiophene-2-aldehyde	190	C5H3BrOS	018791-75-8	64
3	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	46
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	38
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	38





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

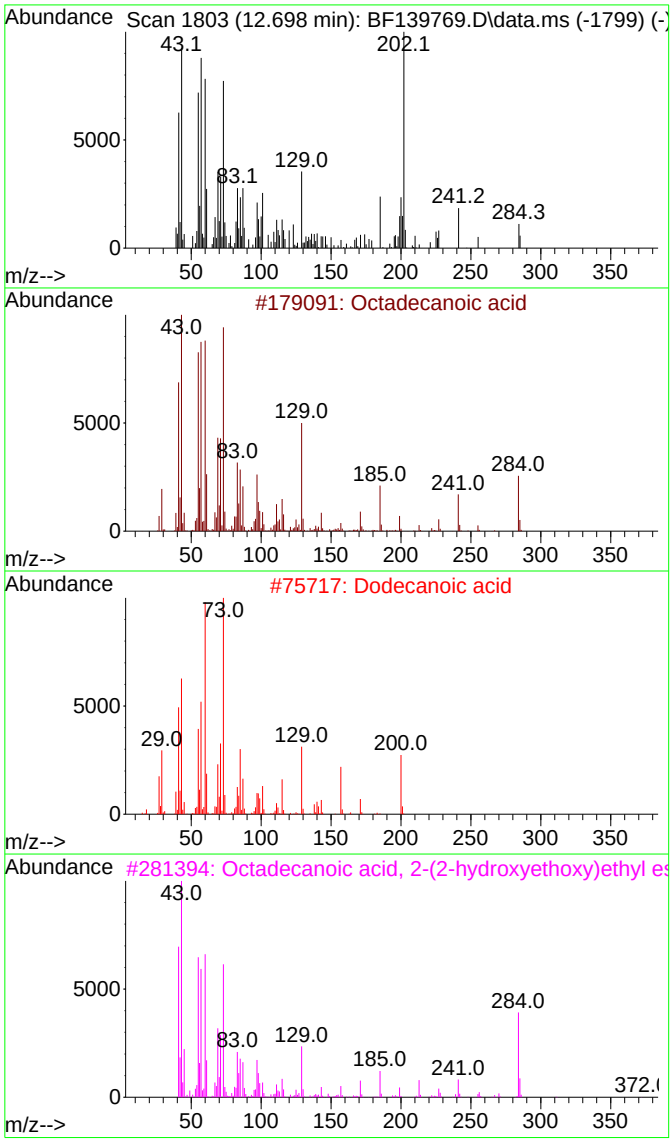
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

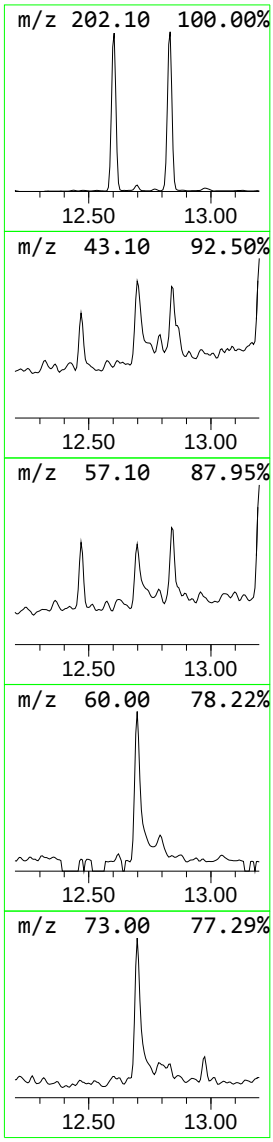
****

Peak Number 7 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.698	2.39 ng	65369	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2	Dodecanoic acid	200	C12H24O2	000143-07-7	64
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	46
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	45
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	43





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Sample : P4364-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-08-0.167-0.667

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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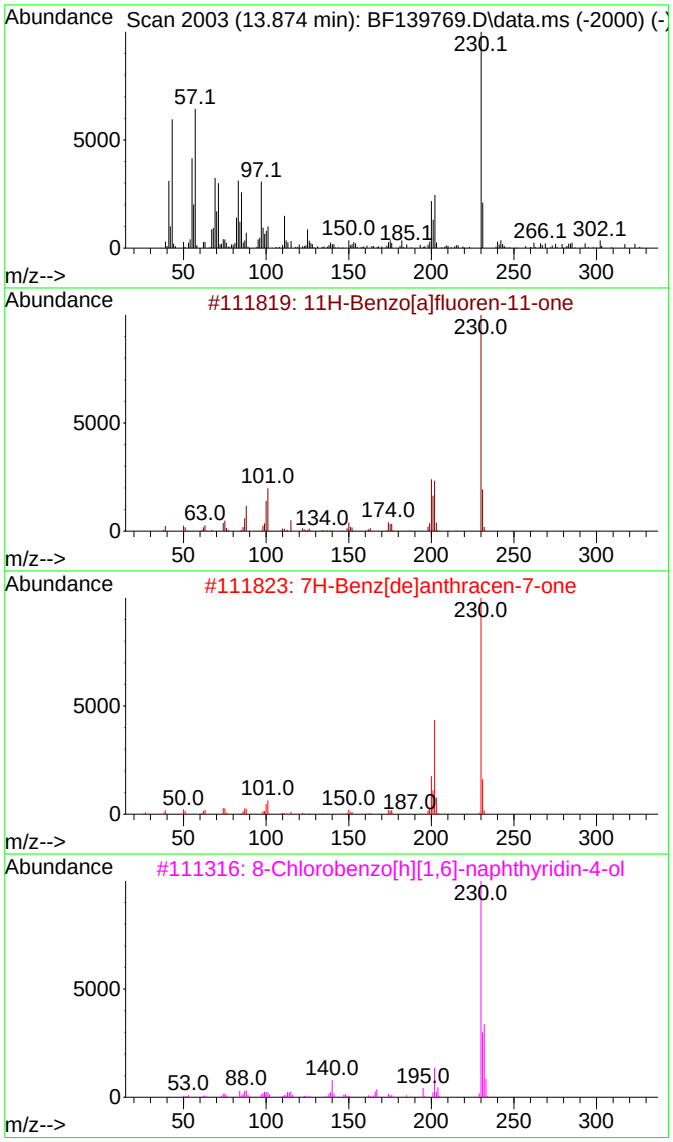
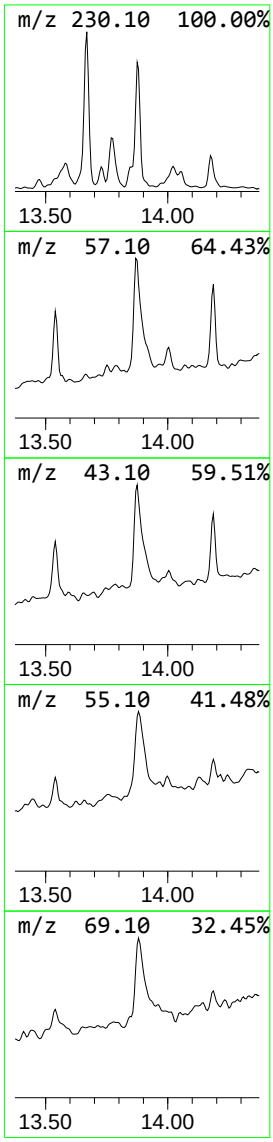
Peak Number 8 11H-Benzo[a]fluoren-11-one Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	3.28 ng	151779	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	93
2	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	64
3	8-Chlorobenzo[h][1,6]-naphthyrid...	230	C12H7ClN2O	025100-26-9	43
4	m-Terphenyl	230	C18H14	000092-06-8	43
5	p-Terphenyl	230	C18H14	000092-94-4	35





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Data File : BF139769.D
Acq On : 11 Oct 2024 12:25
Operator : RC/JU
Sample : P4364-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-08-0.167-0.667

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

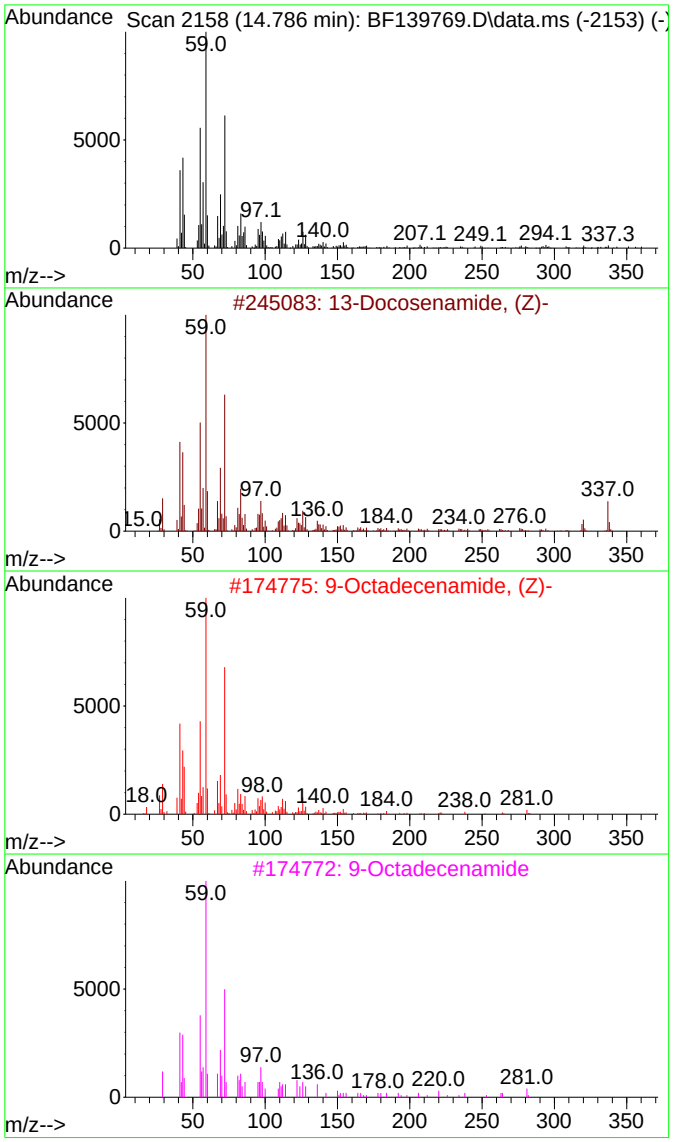
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

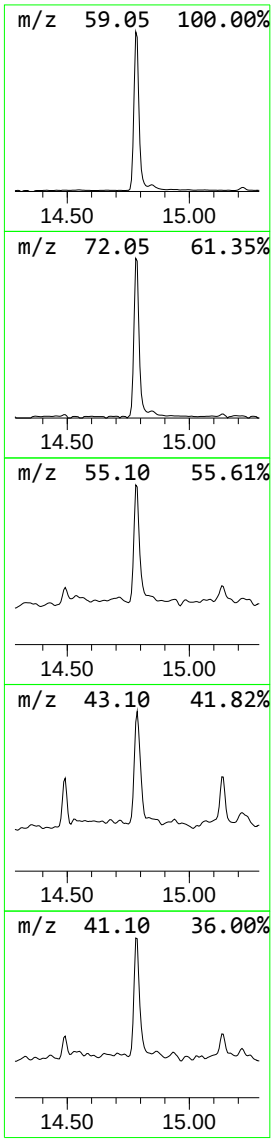
****

Peak Number 9 13-Docosenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	14.27 ng	311171	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
3	9-Octadecenamide	281	C18H35NO	003322-62-1	72
4	Palmitoleamide	253	C16H31NO	106010-22-4	64
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101124\
Data File : BF139769.D
Acq On : 11 Oct 2024 12:25
Operator : RC/JU
Sample : P4364-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-08-0.167-0.667

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

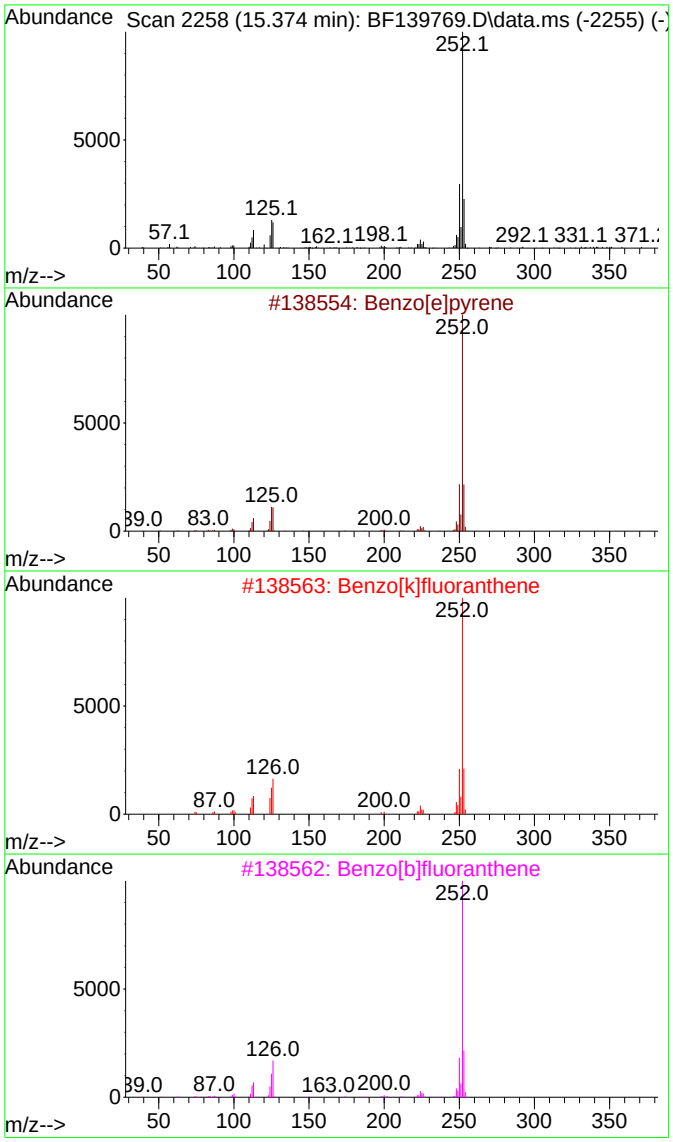
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

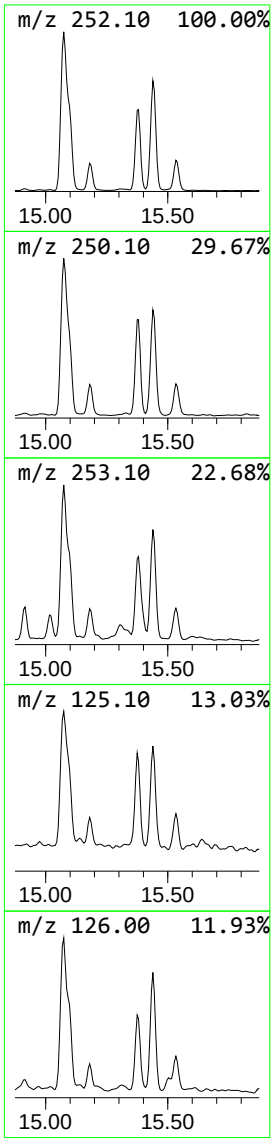
****

Peak Number 10 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.374	5.67 ng	123674	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
4	Perylene	252	C20H12	000198-55-0	94
5	Benzo[a]pyrene	252	C20H12	000050-32-8	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101124\
Data File : BF139769.D
Acq On : 11 Oct 2024 12:25
Operator : RC/JU
Sample : P4364-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-08-0.167-0.667

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...	2.146	98.6	ng	2295120	1	6.869	465752	20.0
2-Pentanone, 4-...	5.081	5.7	ng	132974	1	6.869	465752	20.0
Phthalic acid, ...	10.316	2.2	ng	54706	3	9.898	493519	20.0
Benzophenone	10.616	12.0	ng	295034	3	9.898	493519	20.0
n-Hexadecanoic ...	11.910	13.6	ng	372170	4	11.386	547747	20.0
5-Bromo-2-thiop...	11.998	2.2	ng	60539	4	11.386	547747	20.0
Octadecanoic acid	12.698	2.4	ng	65369	4	11.386	547747	20.0
11H-Benzo[a]flu...	13.874	3.3	ng	151779	5	14.033	924235	20.0
13-Docosenamide...	14.786	14.3	ng	311171	6	15.504	436232	20.0
Benzo[e]pyrene	15.374	5.7	ng	123674	6	15.504	436232	20.0