LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136920.D
Acq On : 03 Jan 2024 21:54
Operator : CG\JU
Sample : 05897-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GHL-SS-31

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136920.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.022	496	499	509	rVB	28420	34488	2.12%	0.213%
2	5.428	564	568	581	rBV	1393231	1369325	84.34%	8.463%
3	5.951	651	657	661	rBV	28082	26525	1.63%	0.164%
4	6.434	734	739	748	rBV	1362117	1373649	84.61%	8.489%
5	6.781	794	798	801	rBV	488382	363456	22.39%	2.246%
6	7.345	889	894	897	rBV	954472	879000	54.14%	5.432%
7	8.057	1011	1015	1017	rBV	597088	464773	28.63%	2.872%
8	8.075	1017	1018	1023	rVB	69824	54006	3.33%	0.334%
9	8.769	1133	1136	1143	rVB	103417	78062	4.81%	0.482%
10	8.869	1147	1153	1158	rVB	33424	27299	1.68%	0.169%
11	9.010	1174	1177	1180	rBV	37871	28498	1.76%	0.176%
12	9.133	1194	1198	1201	rBV	2005793	1564622	96.37%	9.670%
13	9.233	1213	1215	1218	rVB	28849	20002	1.23%	0.124%
14	9.392	1239	1242	1247	rBV3	23562	30573	1.88%	0.189%
15	9.469	1252	1255	1258	rBV	24306	23048	1.42%	0.142%
16	9.586	1273	1275	1279	rBV	26703	25859	1.59%	0.160%
17	9.810	1310	1313	1316	rBV	552372	454112	27.97%	2.806%
18	9.845	1316	1319	1323	rVB	145048	115445	7.11%	0.713%
19	10.016	1342	1348	1353	rBV	136211	133549	8.23%	0.825%
20	10.363	1403	1407	1413	rBV	309045	250500	15.43%	1.548%
21	10.445	1417	1421	1424	rVB	45650	37615	2.32%	0.232%
22	10.604	1442	1448	1457	rBV	866653	816325	50.28%	5.045%
23	10.733	1468	1470	1476	rVB2	24903	25222	1.55%	0.156%
24	10.792	1476	1480	1484	rBV3	12296	20490	1.26%	0.127%
25	10.975	1507	1511	1513	rBV2	21316	24454	1.51%	0.151%
26	11.204	1546	1550	1555	rVB	37935	38654	2.38%	0.239%
27	11.251	1555	1558	1563	rVB2	21867	21386	1.32%	0.132%
28	11.304	1563	1567	1569	rBV	507327	448852	27.65%	2.774%
29	11.327	1569	1571	1577	rVV	601860	535040	32.96%	3.307%
30	11.386	1577	1581	1584	rVV	1881299	1623508	100.00%	10.034%
31	11.439	1588	1590	1592	rVB	26896	20386	1.26%	0.126%
32	11.545	1600	1608	1615	rBV	592451	625464	38.53%	3.865%
33	11.692	1630	1633	1636	rBV	59278	48475	2.99%	0.300%
34	11.722	1636	1638	1640	rBV	21897	23530	1.45%	0.145%
35	11.810	1650	1653	1655	rBV	30283	28036	1.73%	0.173%
36	11.845	1655	1659	1664	rVV2	639937	650185	40.05%	4.018%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136920.D
Acq On : 03 Jan 2024 21:54
Operator : CG\JU
Sample : 05897-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-31

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.886	1664	1666	1669	rVV	109305	97140	5.98%	0.600%
38	11.922	1669	1672	1674	rVV	59002	63219	3.89%	0.391%
39	11.945	1674	1676	1680	rVB	49225	39079	2.41%	0.242%
40	11.986	1680	1683	1686	rBV2	37971	40267	2.48%	0.249%
41	12.022	1686	1689	1691	rVB2	27663	24776	1.53%	0.153%
42	12.110	1702	1704	1707	rVB2	40952	30671	1.89%	0.190%
43	12.251	1725	1728	1732	rVB3	49337	47607	2.93%	0.294%
44	12.398	1749	1753	1759	rVB4	21976	34218	2.11%	0.211%
45	12.522	1771	1774	1777	rBV	244969	241493	14.87%	1.492%
46	12.551	1777	1779	1789	rVB3	86032	137037	8.44%	0.847%
47	12.627	1789	1792	1799	rBV	139441	144039	8.87%	0.890%
48	12.751	1808	1813	1816	rBV2	189547	204727	12.61%	1.265%
49	12.804	1819	1822	1828	rVB4	17355	27647	1.70%	0.171%
50	12.898	1829	1838	1842	rBV	1271442	1195304	73.62%	7.387%
51	13.086	1863	1870	1873	rBV	44388	56762	3.50%	0.351%
52	13.151	1879	1881	1884	rVB	41355	28539	1.76%	0.176%
53	13.633	1960	1963	1966	rBV	28807	24721	1.52%	0.153%
54	13.757	1982	1984	1990	rVB4	33599	40882	2.52%	0.253%
55	13.845	1995	1999	2010	rVB4	48461	97274	5.99%	0.601%
56	13.963	2012	2019	2021	rVV2	405824	501631	30.90%	3.100%
57	13.986	2021	2023	2028	rVB	82533	78434	4.83%	0.485%
58	14.163	2050	2053	2057	rVB	26689	25898	1.60%	0.160%
59	14.433	2096	2099	2103	rVB3	29718	31021	1.91%	0.192%
60	14.739	2149	2151	2154	rVB3	22238	20319	1.25%	0.126%
61	14.815	2161	2164	2167	rVB	29744	30832	1.90%	0.191%
62	15.010	2194	2197	2200	rBV	44137	53799	3.31%	0.332%
63	15.315	2246	2249	2255	rVB	27220	32294	1.99%	0.200%
64	15.380	2257	2260	2266	rVB	40937	49475	3.05%	0.306%
65	15.445	2266	2271	2275	rBV	300744	407813	25.12%	2.520%
66	16.315	2415	2419	2424	rVB2	30201	48453	2.98%	0.299%
67	17.568	2628	2632	2637	rBV8	10425	21030	1.30%	0.130%

Sum of corrected areas: 16180814

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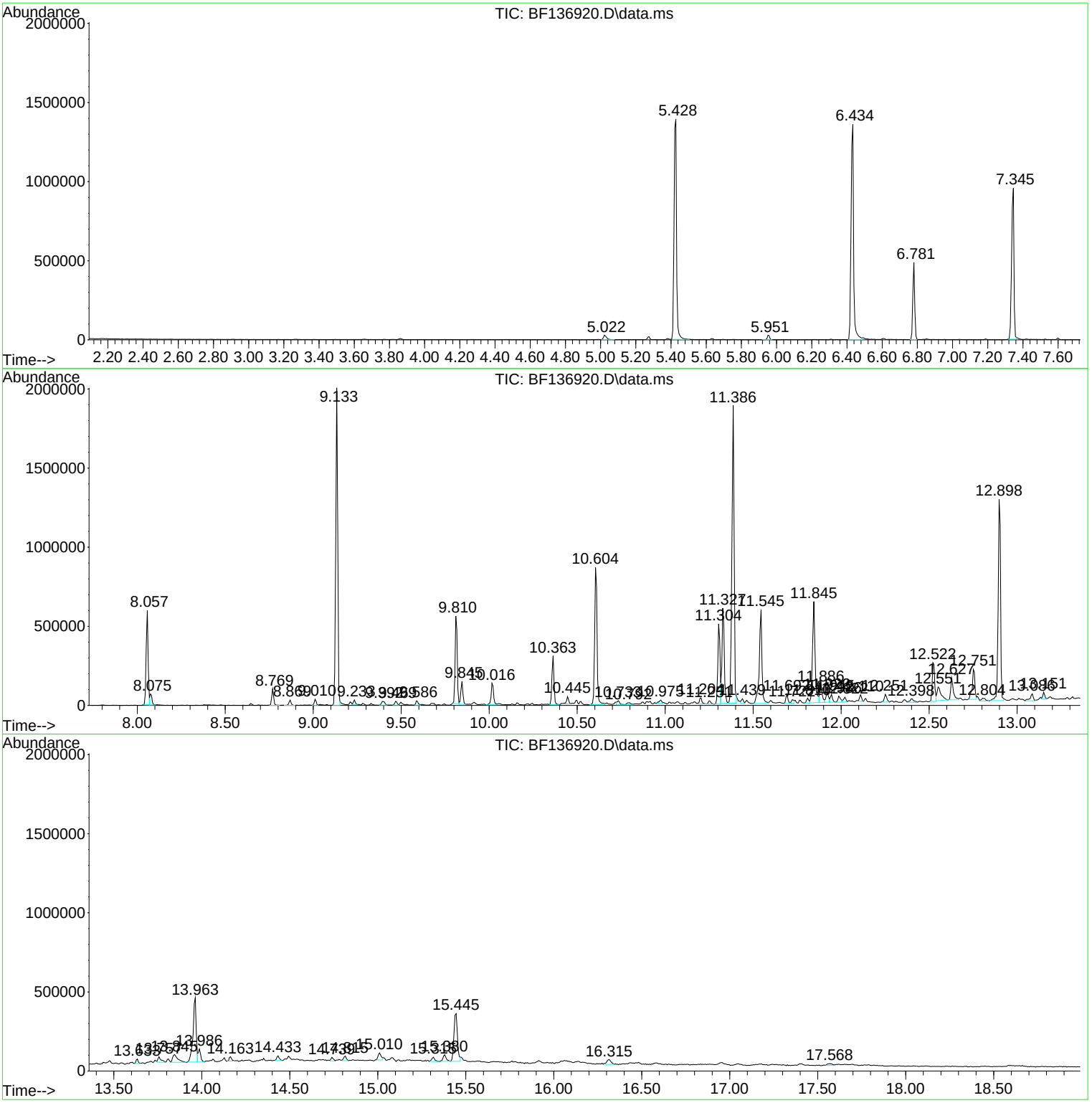
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-31

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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\BF010324\
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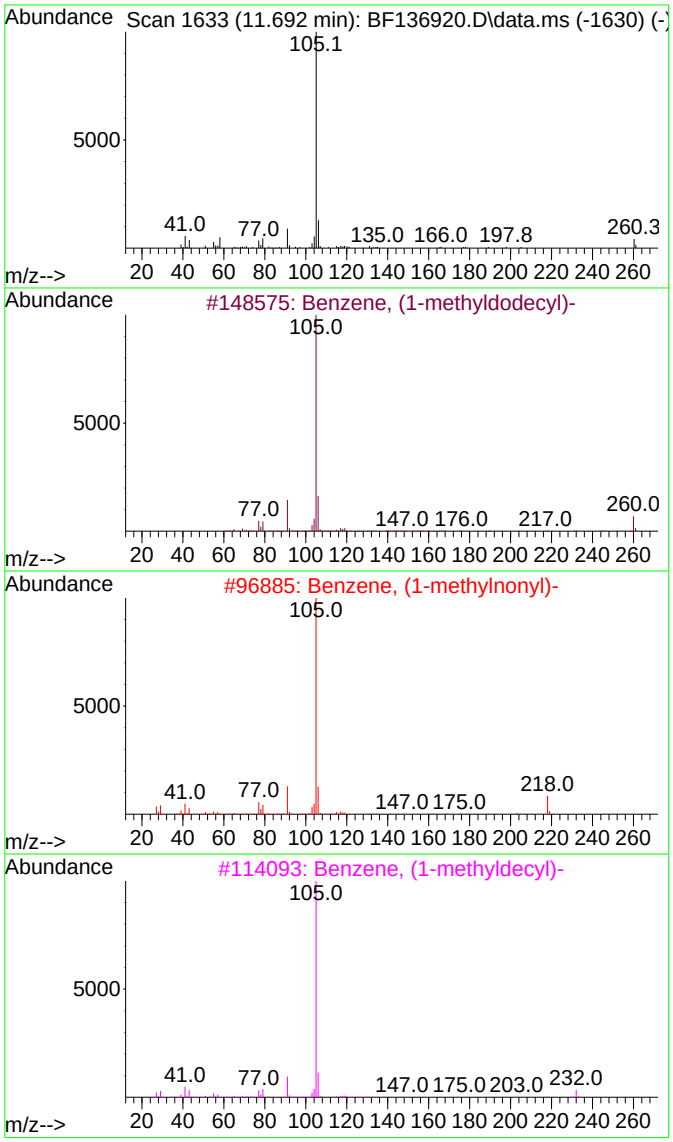
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

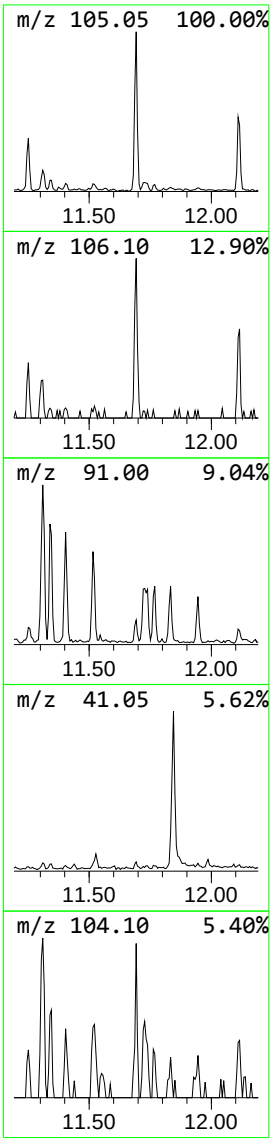
****

Peak Number 1 Benzene, (1-methyldodecyl)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.692	2.16 ng	48475	Phenanthrene-d10	11.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyldodecyl)-	260	C19H32	004534-53-6	81
2	Benzene, (1-methylnonyl)-	218	C16H26	004537-13-7	64
3	Benzene, (1-methyldecyl)-	232	C17H28	004536-88-3	64
4	Benzene, (1-methylundecyl)-	246	C18H30	002719-61-1	64
5	Benzene, (1-methylnonadecyl)-	358	C26H46	002398-66-5	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136920.D
Acq On : 03 Jan 2024 21:54
Operator : CG\JU
Sample : 05897-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-31

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

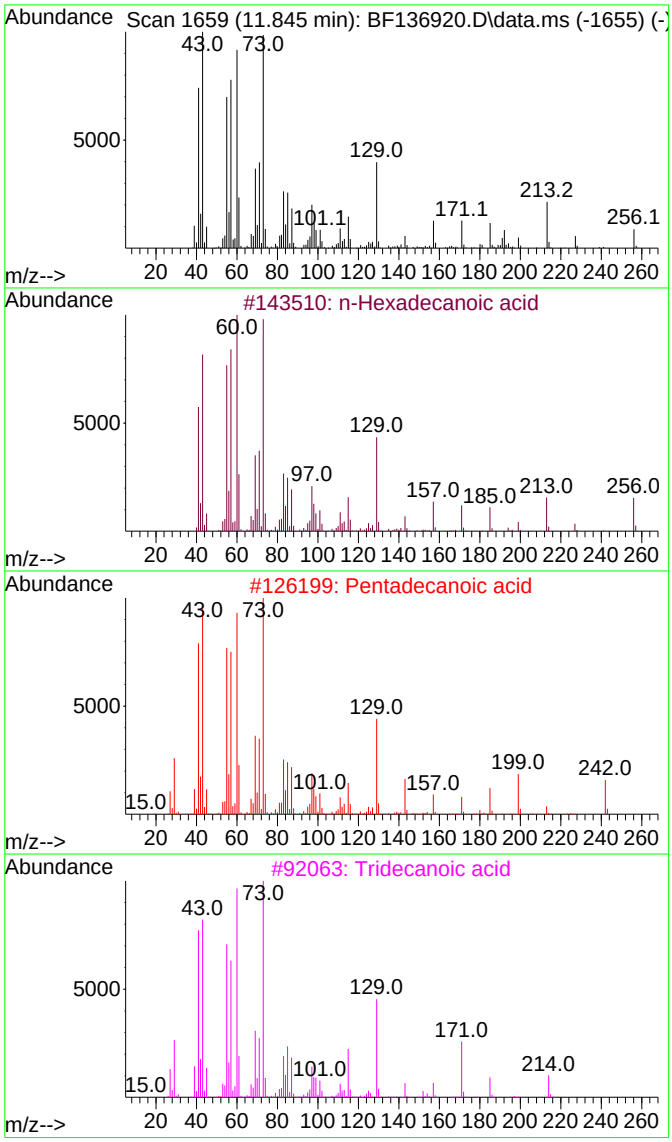
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

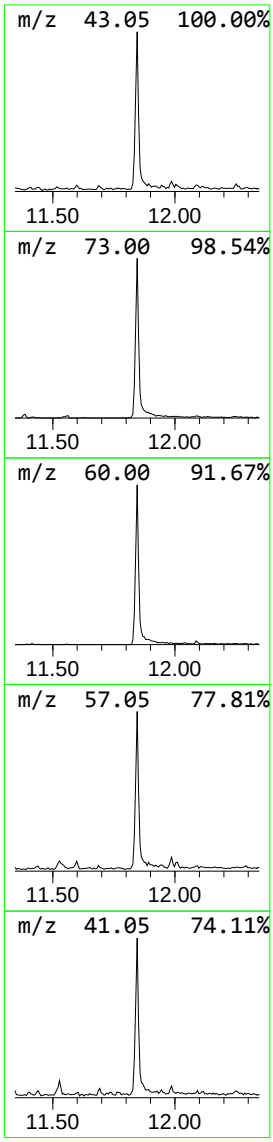
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.845	28.97 ng	650185	Phenanthrene-d10	11.304

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	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136920.D
Acq On : 03 Jan 2024 21:54
Operator : CG\JU
Sample : 05897-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-31

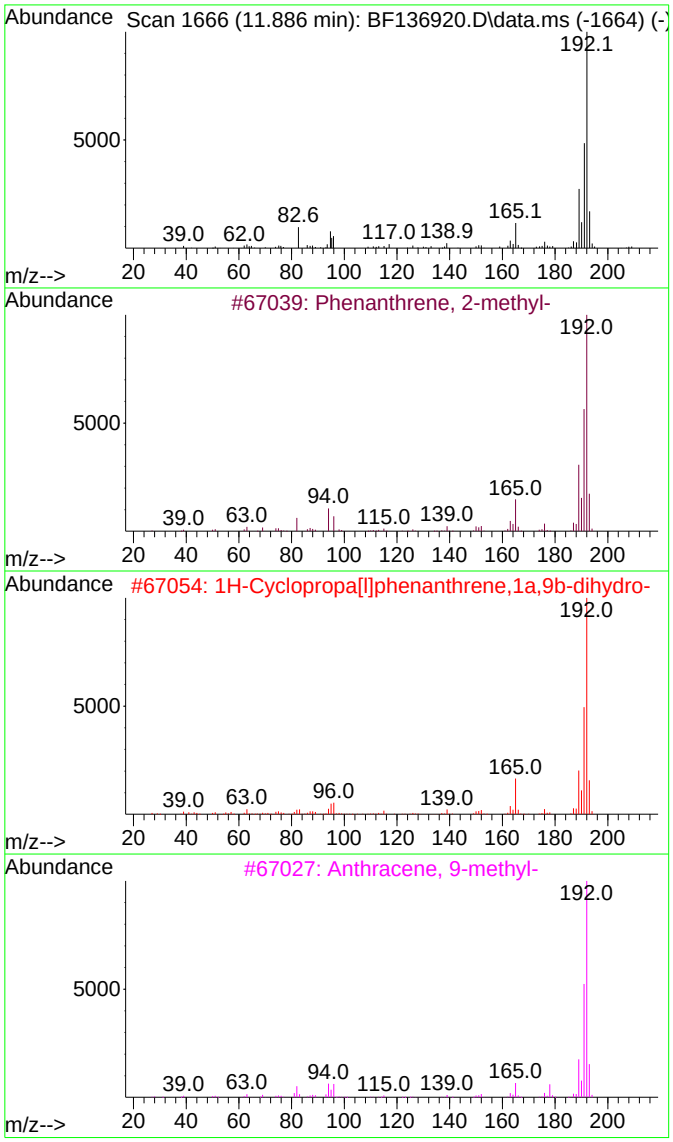
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

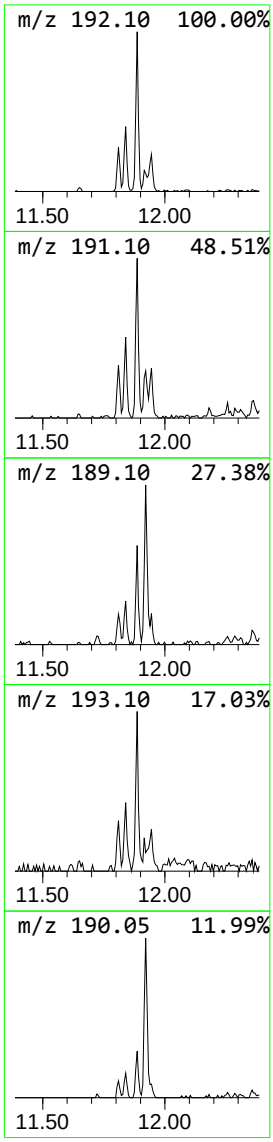
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Phenanthrene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	4.33 ng	97140	Phenanthrene-d10	11.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
2	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	94
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	94
4	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	93
5	Phenanthrene, 9-methyl-	192	C15H12	000883-20-5	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136920.D
Acq On : 03 Jan 2024 21:54
Operator : CG\JU
Sample : 05897-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-31

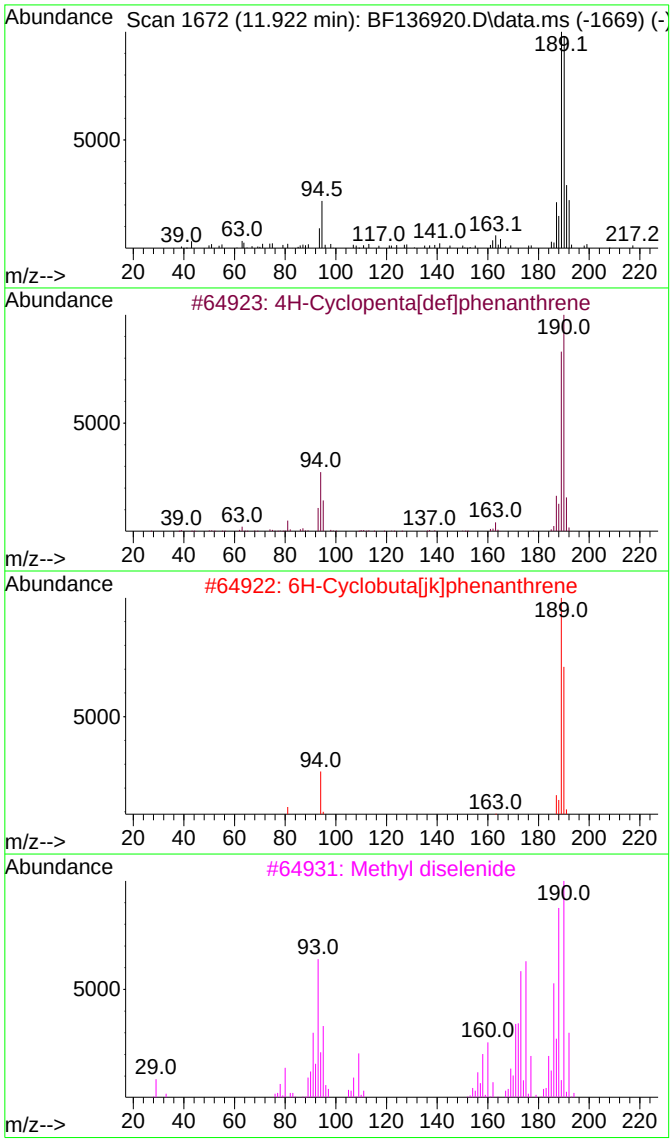
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

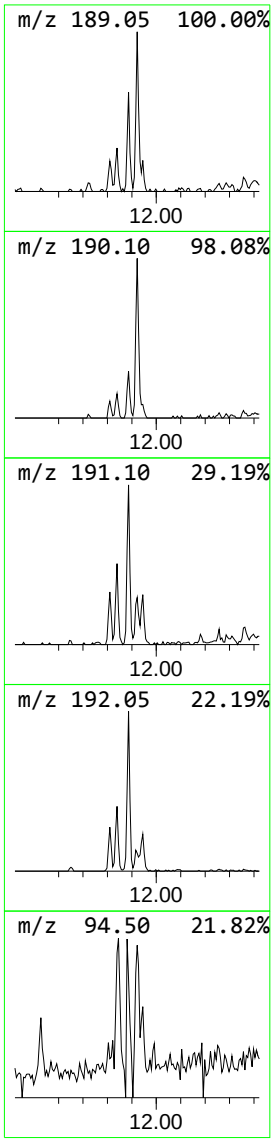
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	2.82 ng	63219	Phenanthrene-d10	11.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	83
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
3	Methyl diselenide	190	C2H6Se2	007101-31-7	43
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
5	Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136920.D
Acq On : 03 Jan 2024 21:54
Operator : CG\JU
Sample : 05897-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-31

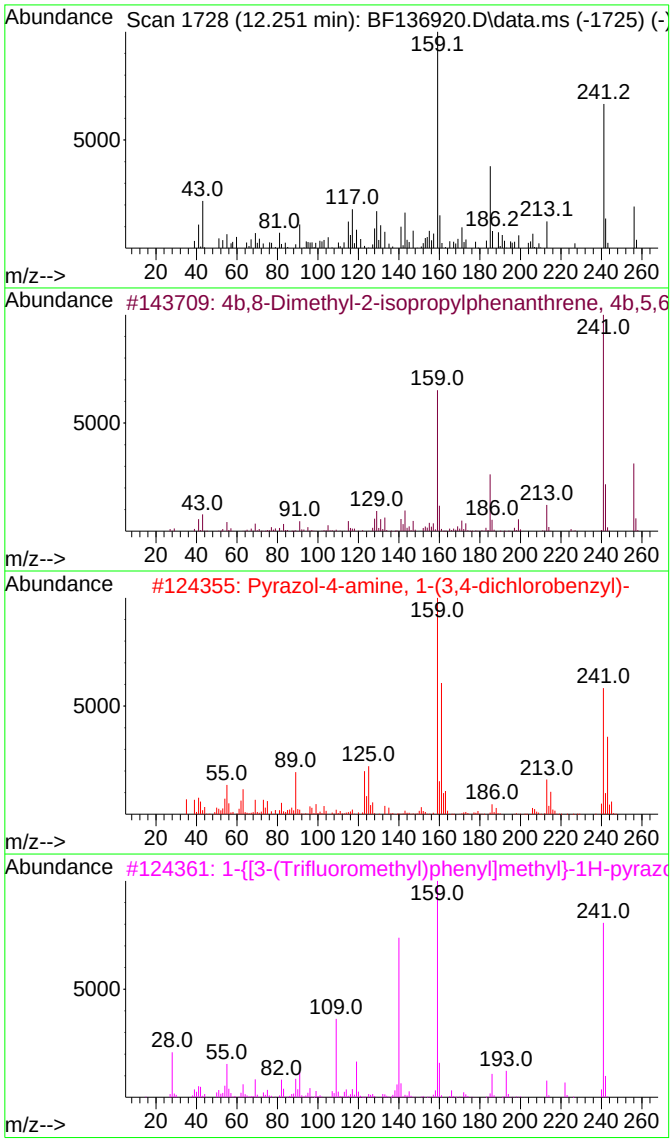
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

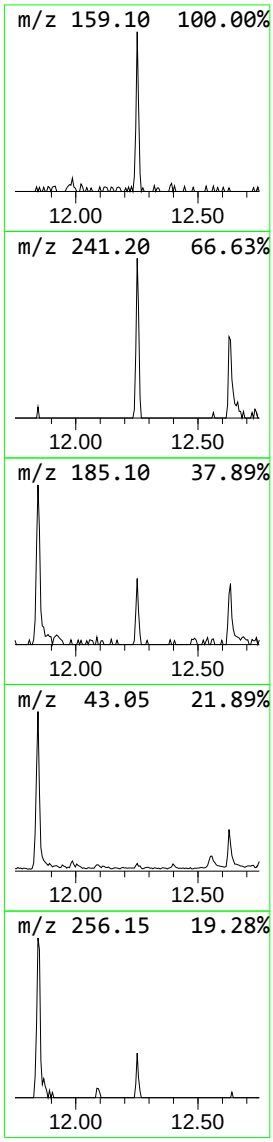
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4b,8-Dimethyl-2-isopropylph... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.251	2.12 ng	47607	Phenanthrene-d10	11.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4b,8-Dimethyl-2-isopropylphenant...	256	C19H28	1000197-14-1	98
2	Pyrazol-4-amine, 1-(3,4-dichloro...	241	C10H9Cl2N3	1000273-77-4	53
3	1-{[3-(Trifluoromethyl)phenyl]me...	241	C11H10F3N3	1002033-51-3	50
4	s-Indacen-1(2H)-one, 3,5,6,7-tet...	256	C18H24O	038754-94-8	42
5	Cyclohexanecarboxylic acid, 1-ph...	204	C13H16O2	001135-67-7	30





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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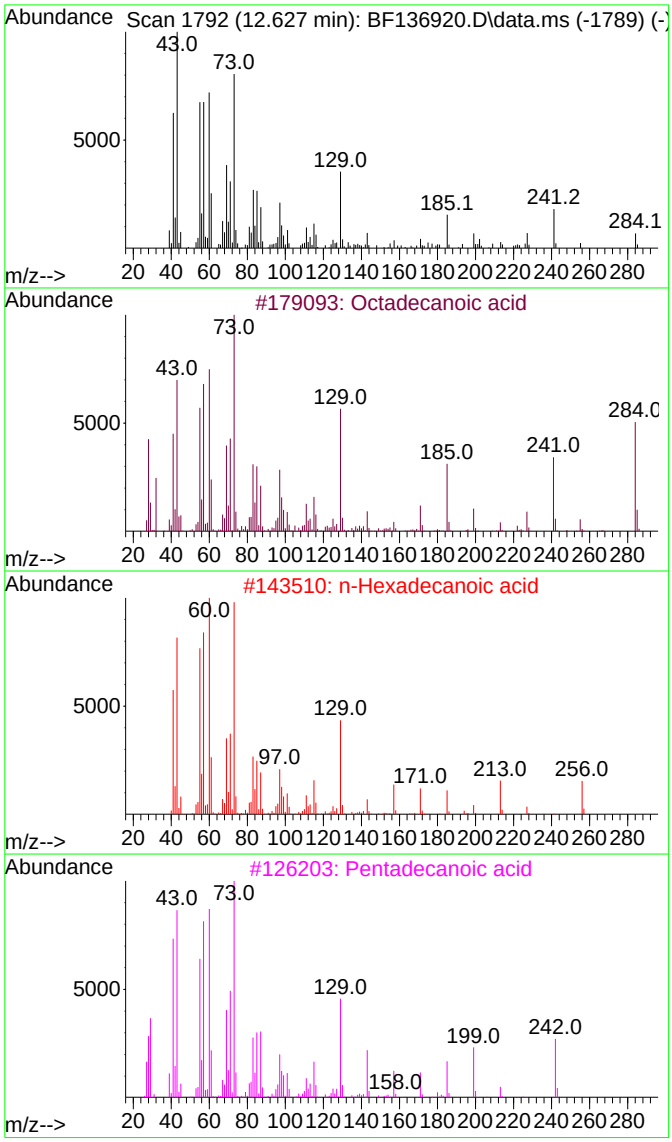
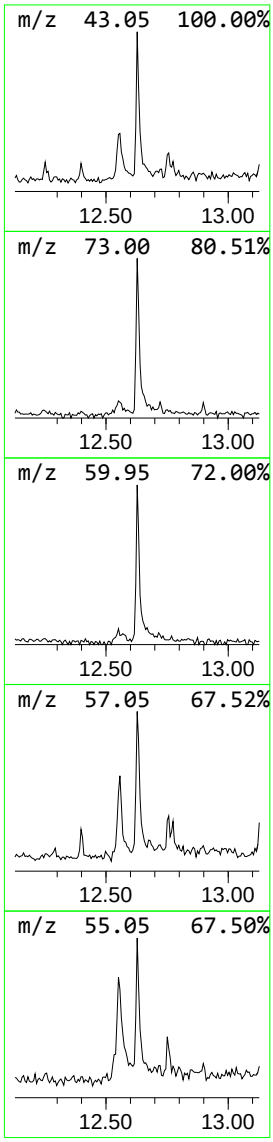
Peak Number 6 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.627	6.42 ng	144039	Phenanthrene-d10	11.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136920.D
Acq On : 03 Jan 2024 21:54
Operator : CG\JU
Sample : 05897-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-31

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

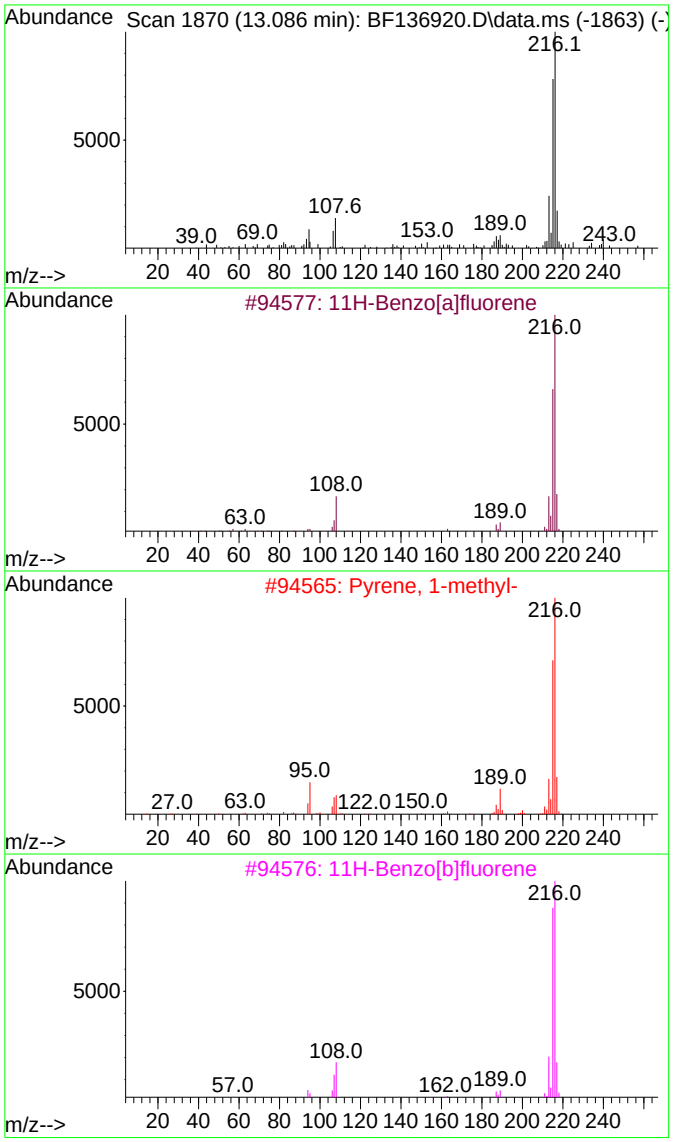
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

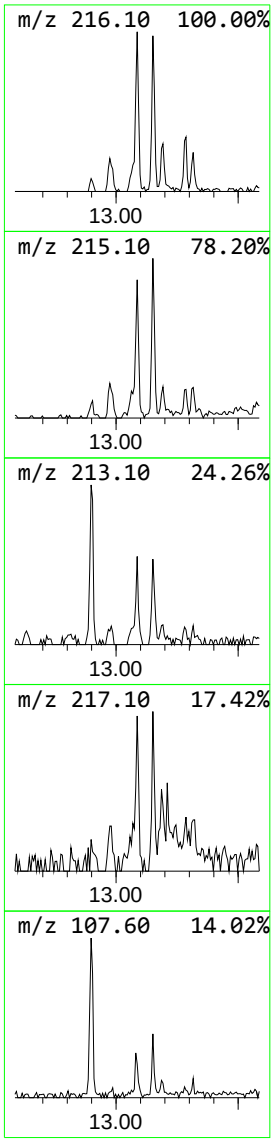
****

Peak Number 7 11H-Benzo[a]fluorene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.086	2.26 ng	56762	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	93
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	91
3	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	90
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	81





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Acq On : 03 Jan 2024 21:54
Operator : CG\JU
Sample : 05897-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-31

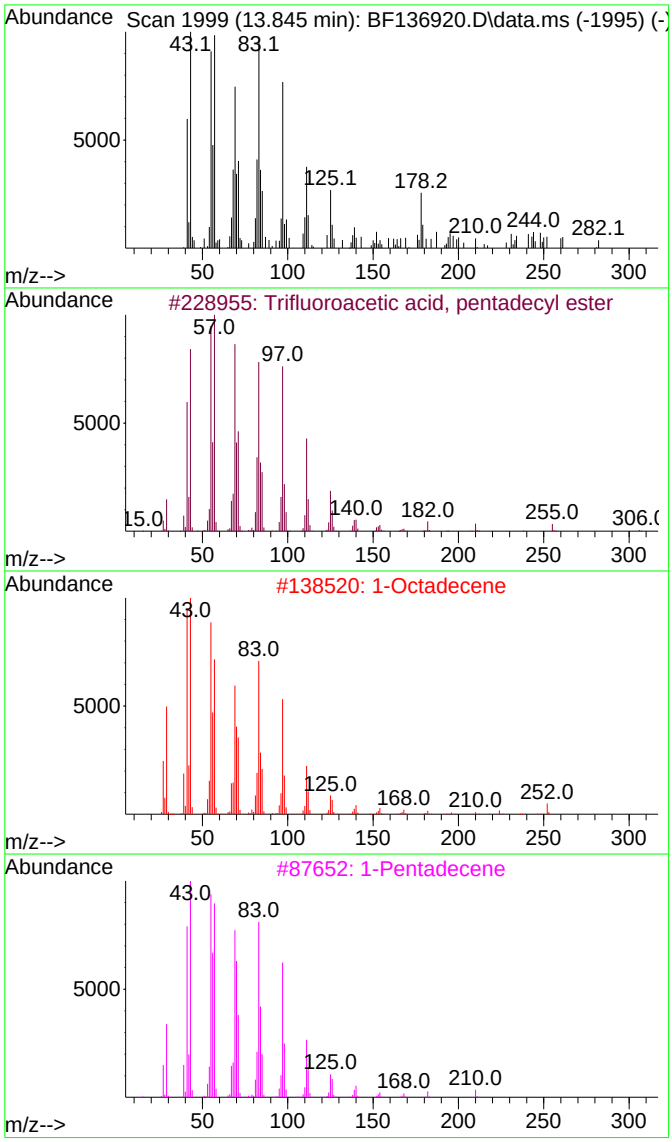
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

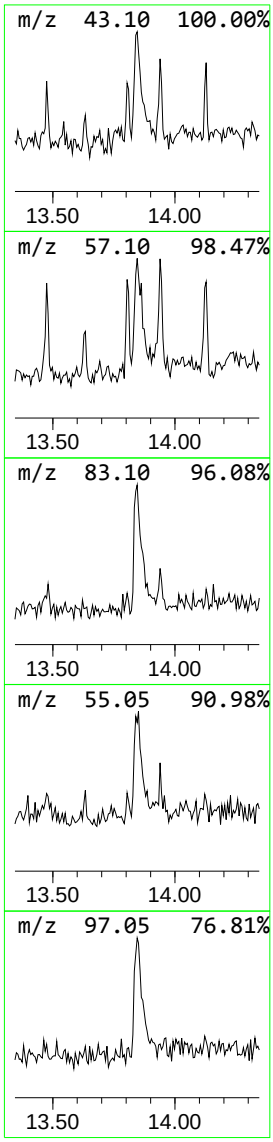
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Trifluoroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	3.88 ng	97274	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
2	1-Octadecene	252	C18H36	000112-88-9	91
3	1-Pentadecene	210	C15H30	013360-61-7	90
4	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	87
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136920.D
Acq On : 03 Jan 2024 21:54
Operator : CG\JU
Sample : 05897-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-31

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

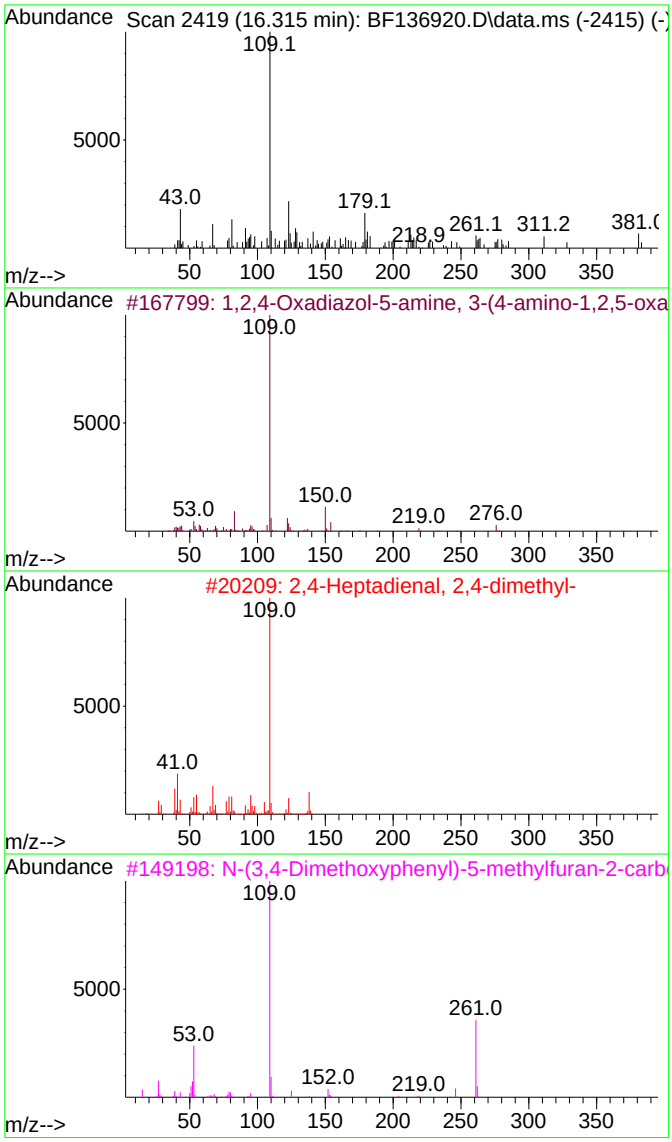
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

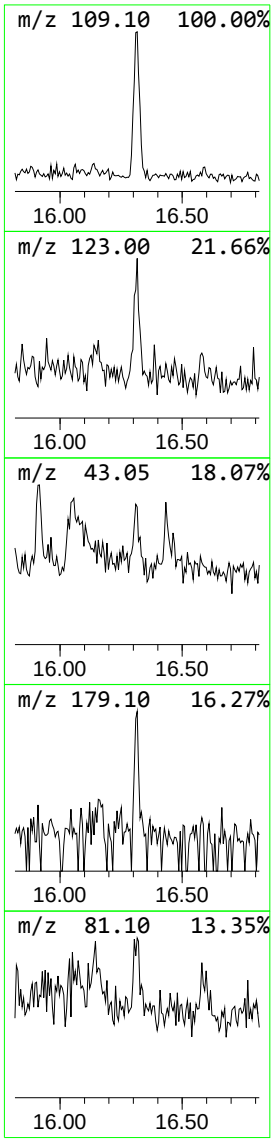
****

Peak Number 9 unknown16.315 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.315	2.38 ng	48453	Perylene-d12	15.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Oxadiazol-5-amine, 3-(4-am...	276	C11H9FN6O2	1000351-27-3	47
2	2,4-Heptadienal, 2,4-dimethyl-	138	C9H14O	042452-48-2	47
3	N-(3,4-Dimethoxyphenyl)-5-methyl...	261	C14H15NO4	1000436-26-2	47
4	6,6-Dimethylhepta-2,4-diene	124	C9H16	1000195-03-3	46
5	4-Pentyloxyaniline	179	C11H17NO	039905-50-5	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136920.D
Acq On : 03 Jan 2024 21:54
Operator : CG\JU
Sample : 05897-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-31

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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
Benzene, (1-met...	11.692	2.2	ng	48475	4	11.304	448852	20.0
n-Hexadecanoic ...	11.845	29.0	ng	650185	4	11.304	448852	20.0
Phenanthrene, 2...	11.886	4.3	ng	97140	4	11.304	448852	20.0
4H-Cyclopenta[d...	11.922	2.8	ng	63219	4	11.304	448852	20.0
4b,8-Dimethyl-2...	12.251	2.1	ng	47607	4	11.304	448852	20.0
Octadecanoic acid	12.627	6.4	ng	144039	4	11.304	448852	20.0
11H-Benzo[a]flu...	13.086	2.3	ng	56762	5	13.963	501631	20.0
Trifluoroacetic...	13.845	3.9	ng	97274	5	13.963	501631	20.0
unknown16.315	16.315	2.4	ng	48453	6	15.445	407813	20.0