LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031424\
Data File : BF137598.D
Acq On : 14 Mar 2024 19:00
Operator : CG\JU
Sample : P1744-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT-3488

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-BF022924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137598.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.334	548	552	574	rBV	2199737	2186747	51.18%	7.580%
2	6.357	722	726	748	rBV	2921509	3079905	72.09%	10.676%
3	6.722	785	788	801	rBV	843968	855707	20.03%	2.966%
4	7.287	881	884	909	rBV	1756363	1669228	39.07%	5.786%
5	8.004	1003	1006	1019	rBV	1230960	1128967	26.43%	3.914%
6	9.081	1185	1189	1193	rBV	4496663	4272273	100.00%	14.810%
7	9.757	1300	1304	1308	rBV	1573833	1272430	29.78%	4.411%
8	10.545	1434	1438	1455	rBV	2785836	2567991	60.11%	8.902%
9	11.045	1520	1523	1528	rBV2	76792	100303	2.35%	0.348%
10	11.239	1552	1556	1558	rBV	1410544	1170182	27.39%	4.056%
11	11.263	1558	1560	1567	rVB	483242	418673	9.80%	1.451%
12	11.739	1638	1641	1644	rBV	77864	75365	1.76%	0.261%
13	11.774	1644	1647	1653	rVV2	210900	297139	6.96%	1.030%
14	11.851	1657	1660	1662	rVV	119012	131089	3.07%	0.454%
15	11.874	1662	1664	1668	rVB	64943	63237	1.48%	0.219%
16	12.063	1694	1696	1703	rVB	48167	56440	1.32%	0.196%
17	12.286	1731	1734	1737	rBV	63108	68742	1.61%	0.238%
18	12.327	1737	1741	1746	rVB4	43473	72070	1.69%	0.250%
19	12.374	1746	1749	1752	rBV	52713	56254	1.32%	0.195%
20	12.445	1758	1761	1766	rBV	511115	491379	11.50%	1.703%
21	12.674	1795	1800	1803	rBV	541615	523108	12.24%	1.813%
22	12.827	1821	1826	1829	rBV	4126209	3803294	89.02%	13.184%
23	12.898	1835	1838	1842	rVB2	35389	46418	1.09%	0.161%
24	13.074	1863	1868	1870	rBV3	35555	52267	1.22%	0.181%
25	13.110	1871	1874	1877	rVB2	53527	53137	1.24%	0.184%
26	13.204	1886	1890	1893	rBV	110263	119485	2.80%	0.414%
27	13.516	1940	1943	1947	rVB	45963	57109	1.34%	0.198%
28	13.627	1958	1962	1964	rBV	37964	48674	1.14%	0.169%
29	13.739	1976	1981	1989	rBV3	129211	270010	6.32%	0.936%
30	13.874	1997	2004	2007	rBV2	950049	1190836	27.87%	4.128%
31	13.898	2007	2008	2015	rVB	222452	175850	4.12%	0.610%
32	14.380	2087	2090	2098	rVB4	89771	157257	3.68%	0.545%
33	14.510	2109	2112	2116	rBV	66793	80285	1.88%	0.278%
34	14.715	2144	2147	2153	rBV	94486	117004	2.74%	0.406%
35	14.892	2173	2177	2180	rBV	214225	309024	7.23%	1.071%
36	15.174	2222	2225	2230	rVB	153182	170176	3.98%	0.590%

LSC Area Percent Report

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Instrument :
BNA_F
ClientSampleId :
RT-3488

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-BF022924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.233	2232	2235	2240	rBV	155990	187897	4.40%	0.651%
38	15.292	2241	2245	2250	rBV	739022	939842	22.00%	3.258%
39	16.268	2407	2411	2420	rVB7	58740	111543	2.61%	0.387%
40	16.680	2476	2481	2492	rVB2	83113	180213	4.22%	0.625%
41	17.092	2546	2551	2558	rBV	68854	146167	3.42%	0.507%
42	17.251	2572	2578	2586	rBV	26730	73984	1.73%	0.256%

Sum of corrected areas: 28847701

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Instrument :
BNA_F
ClientSampleId :
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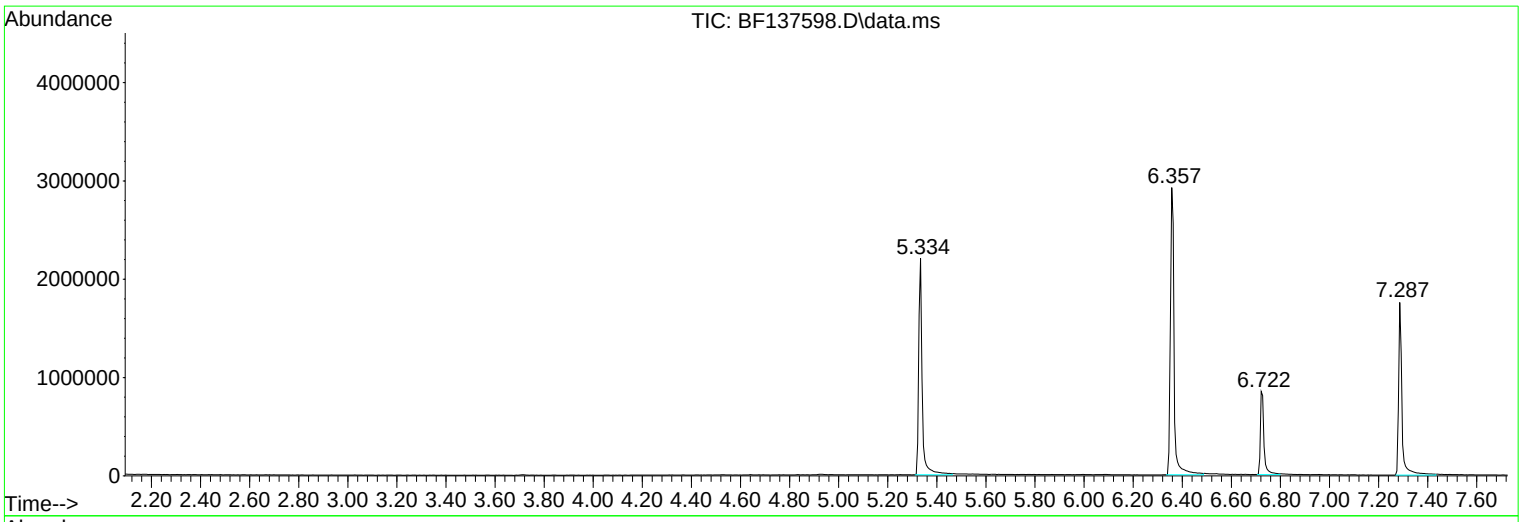
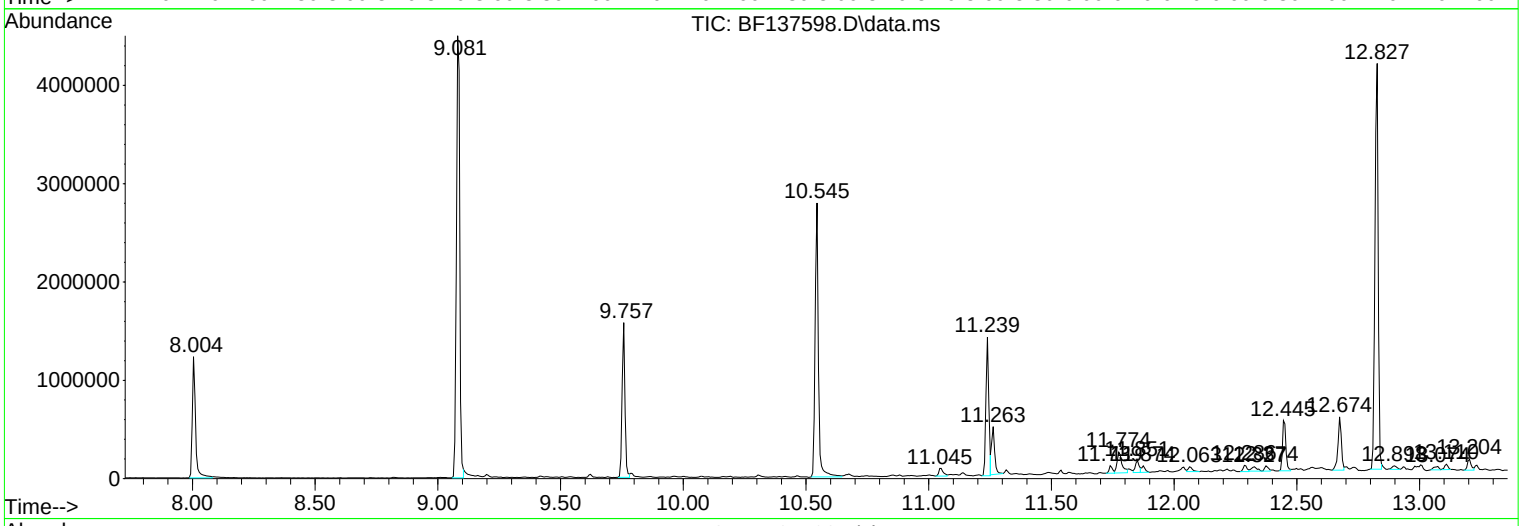
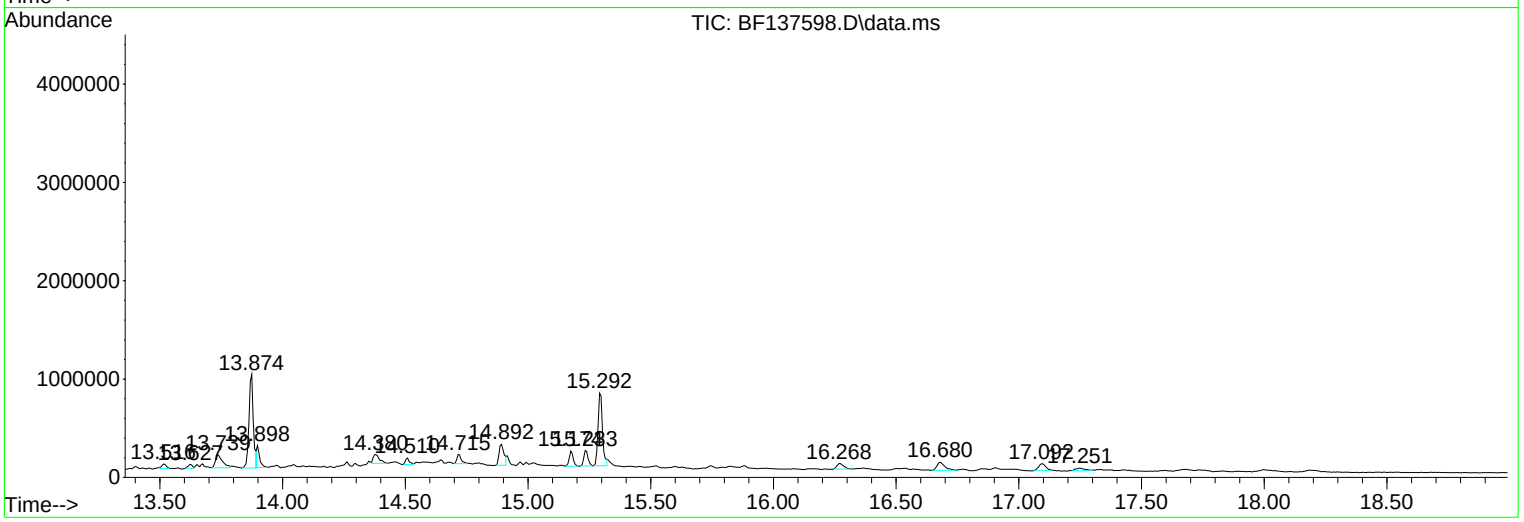
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Data File : BF137598.D
Acq On : 14 Mar 2024 19:00
Operator : CG\JU
Sample : P1744-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

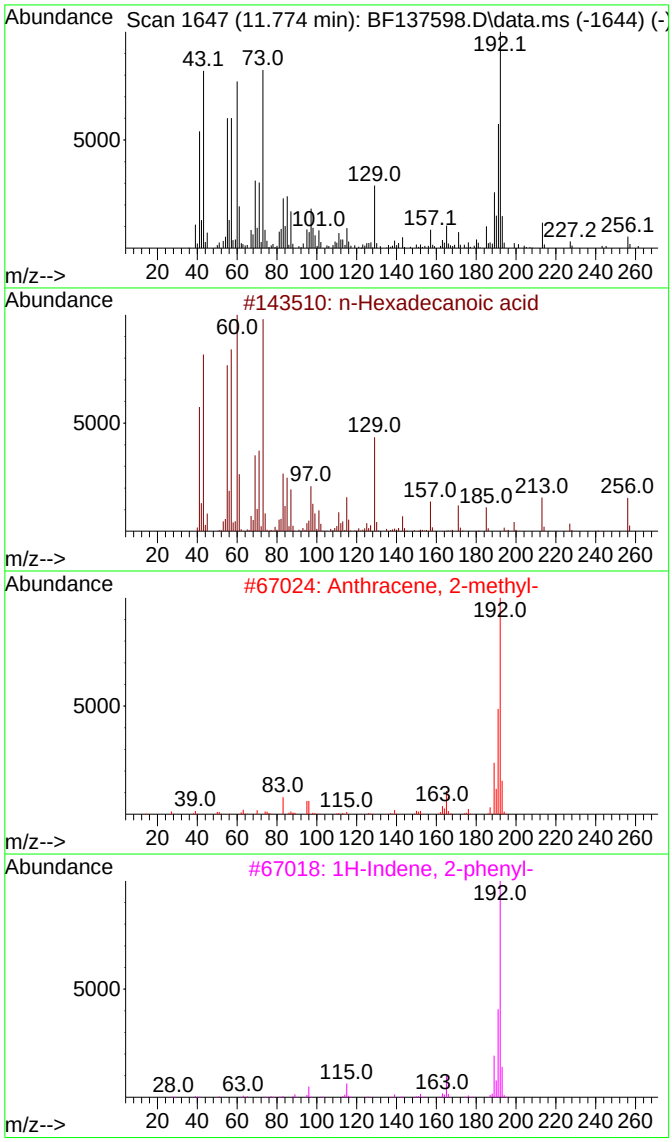
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

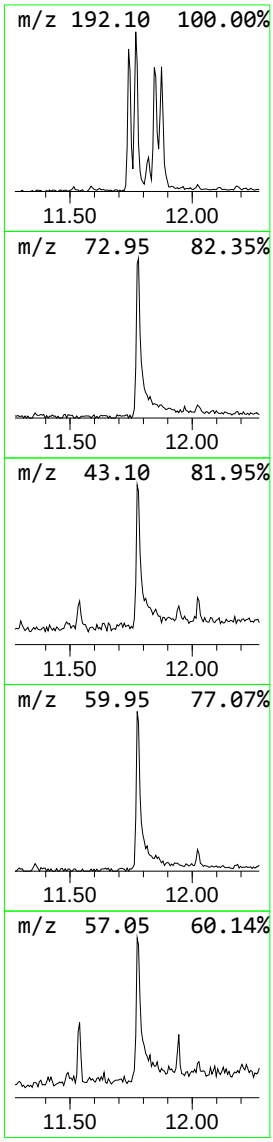
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.775	5.08 ng	297139	Phenanthrene-d10	11.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	86
3	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	83
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	80
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	80





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Acq On : 14 Mar 2024 19:00
Operator : CG\JU
Sample : P1744-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-3488

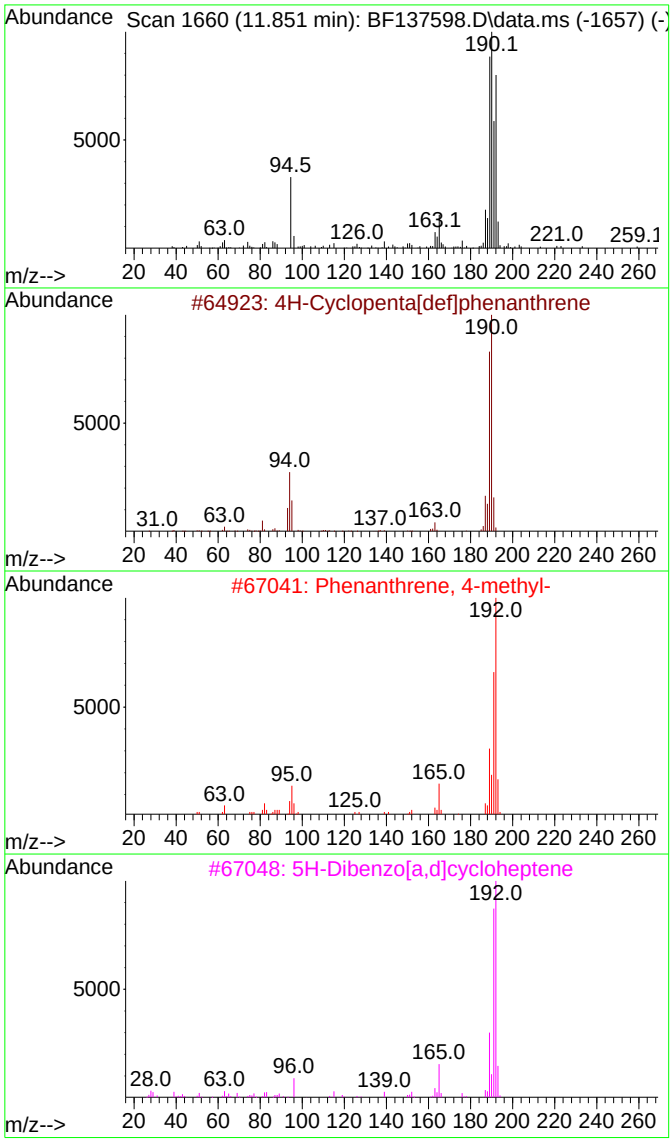
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

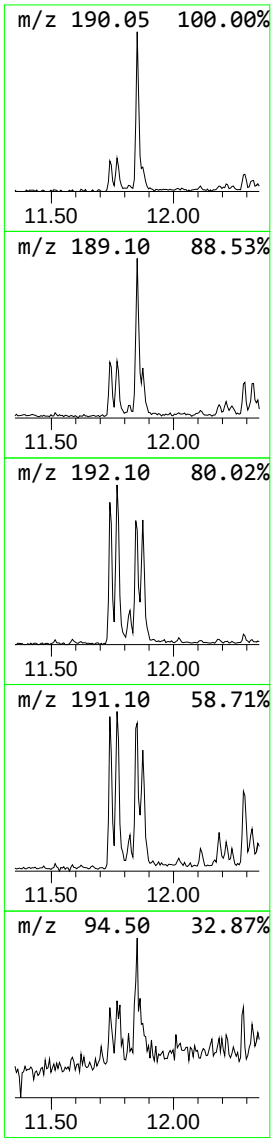
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	2.24 ng	131089	Phenanthrene-d10	11.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	60
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	42
3	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	42
4	1a,9b-Dihydro-1H-cyclopropa[a]an...	192	C15H12	006109-24-6	42
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	38





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Data File : BF137598.D
Acq On : 14 Mar 2024 19:00
Operator : CG\JU
Sample : P1744-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-3488

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.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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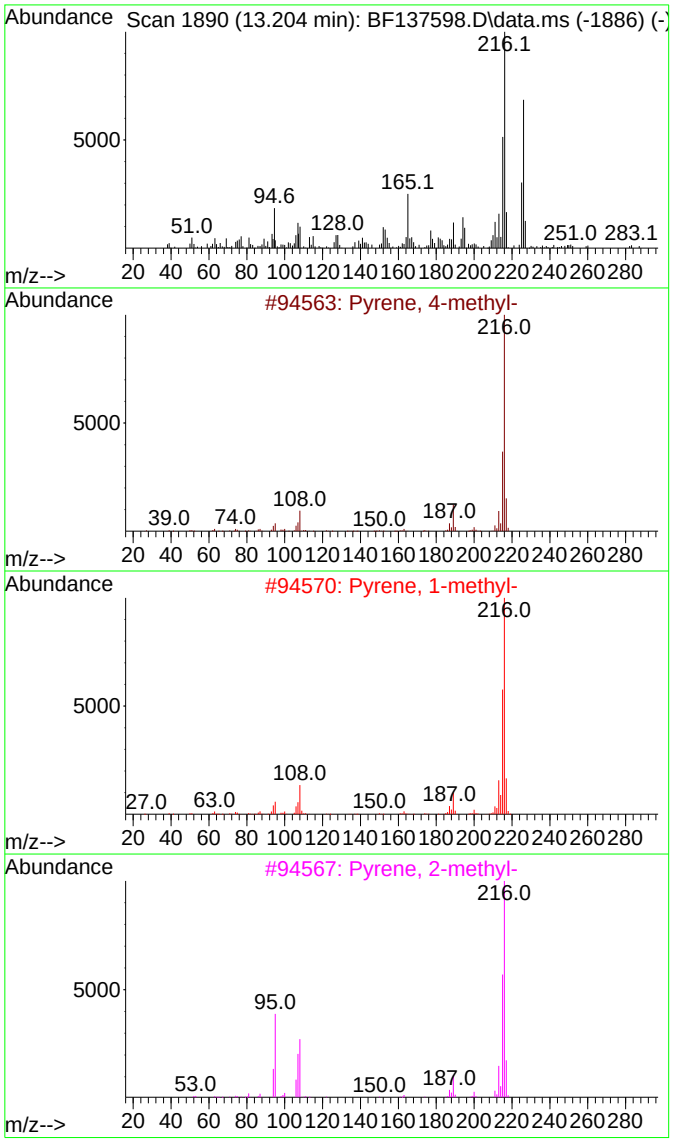
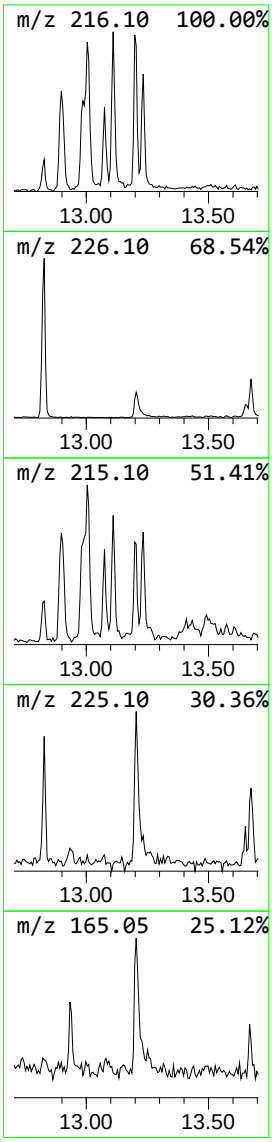
Peak Number 3 Pyrene, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.204	2.01 ng	119485	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 4-methyl-	216	C17H12	003353-12-6	83
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	64
3	Pyrene, 2-methyl-	216	C17H12	003442-78-2	55
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	50
5	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	49





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Operator : CG\JU
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.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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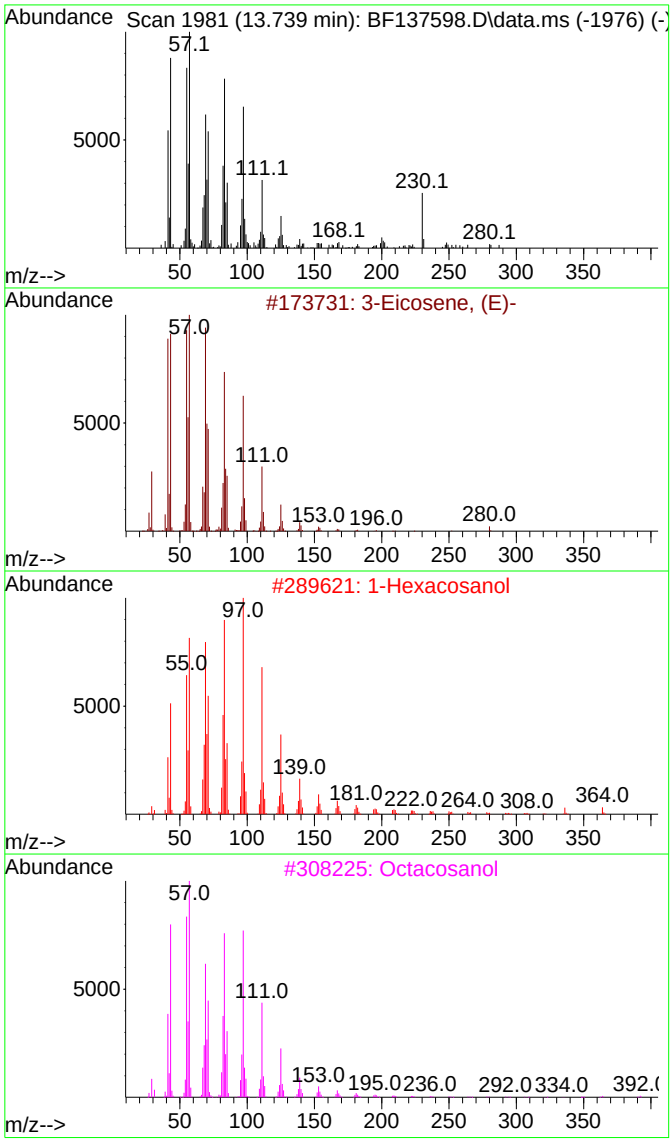
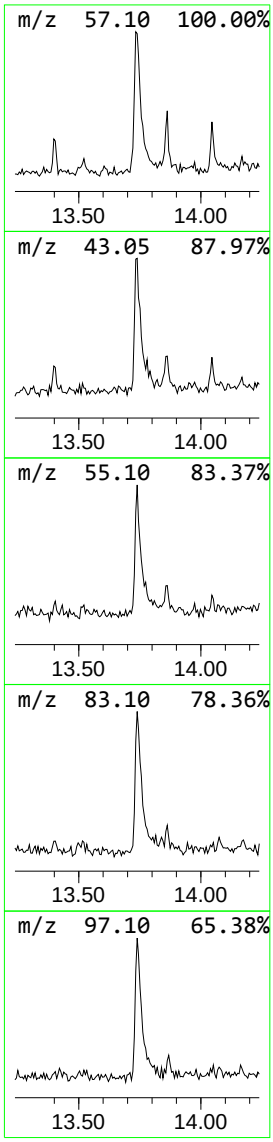
Peak Number 4 3-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.739	4.53 ng	270010	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	92
2	1-Hexacosanol	382	C26H54O	000506-52-5	90
3	Octacosanol	410	C28H58O	000557-61-9	90
4	1-Heptacosanol	396	C27H56O	002004-39-9	90
5	1-Heneicosanol	312	C21H44O	015594-90-8	87





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Data File : BF137598.D
Acq On : 14 Mar 2024 19:00
Operator : CG\JU
Sample : P1744-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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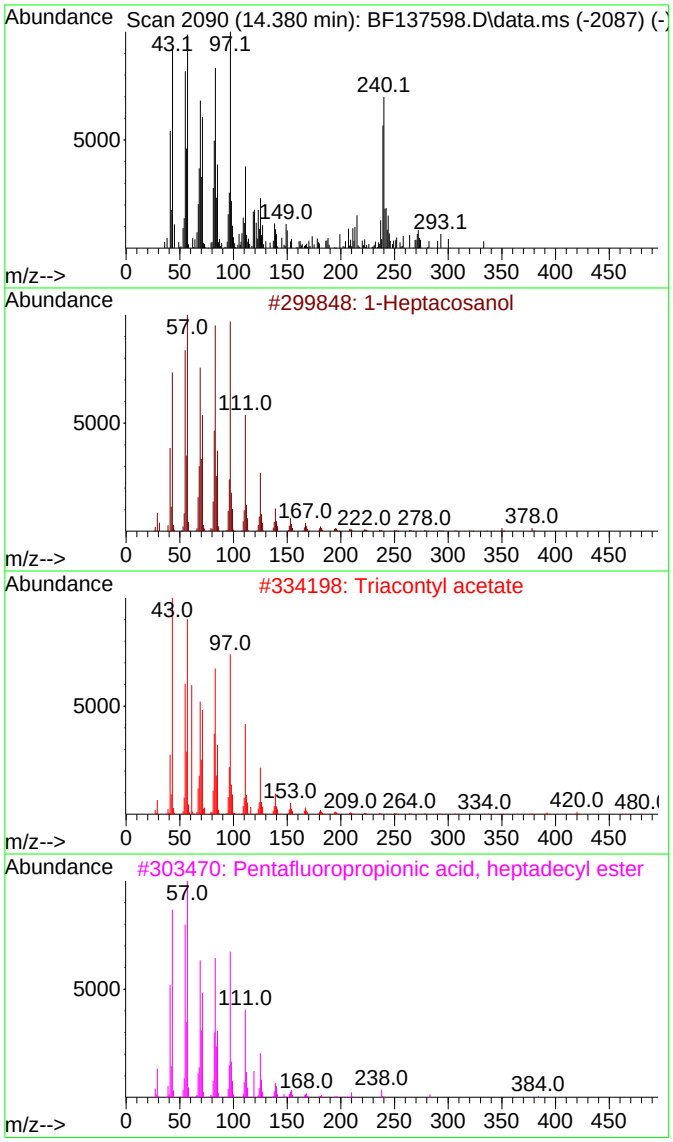
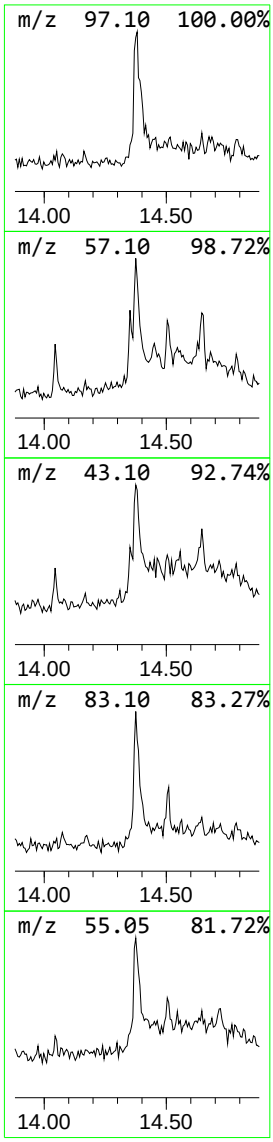
****

Peak Number 5 1-Heptacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.380	2.64 ng	157257	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	83
2	Triacontyl acetate	480	C32H64O2	041755-58-2	70
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	60
4	1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	55
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	53





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Sample : P1744-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.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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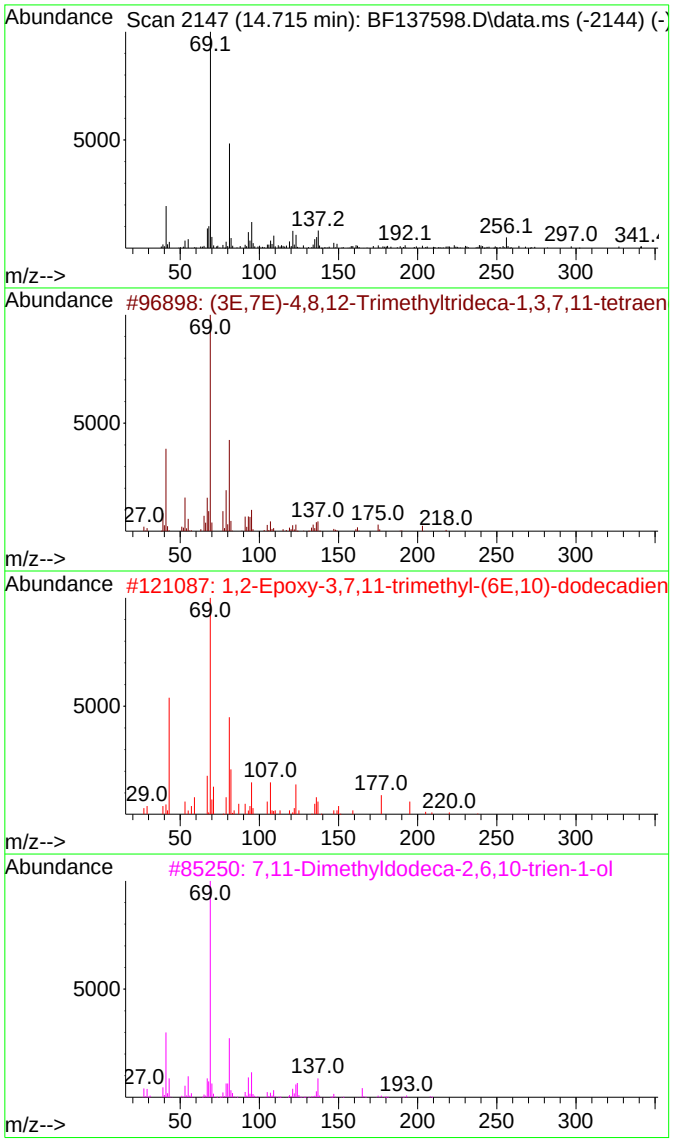
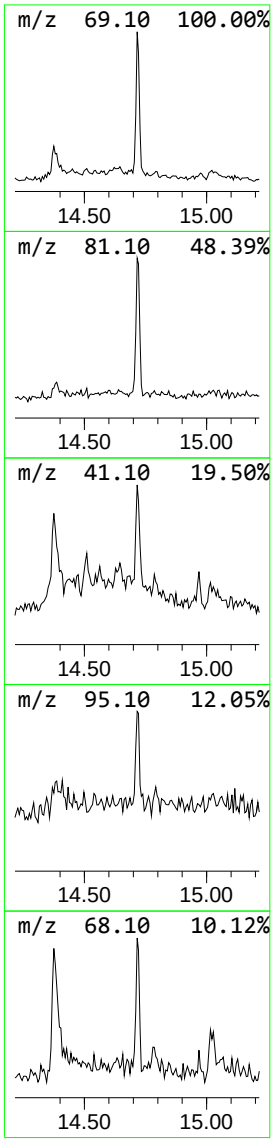
Peak Number 6 (3E,7E)-4,8,12-Trimethyltri... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.716	2.49 ng	117004	Perylene-d12	15.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3E,7E)-4,8,12-Trimethyltrideca-...	218	C16H26	062235-06-7	80
2	1,2-Epoxy-3,7,11-trimethyl-(6E,1...	238	C15H26O2	1000432-46-2	64
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
4	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64





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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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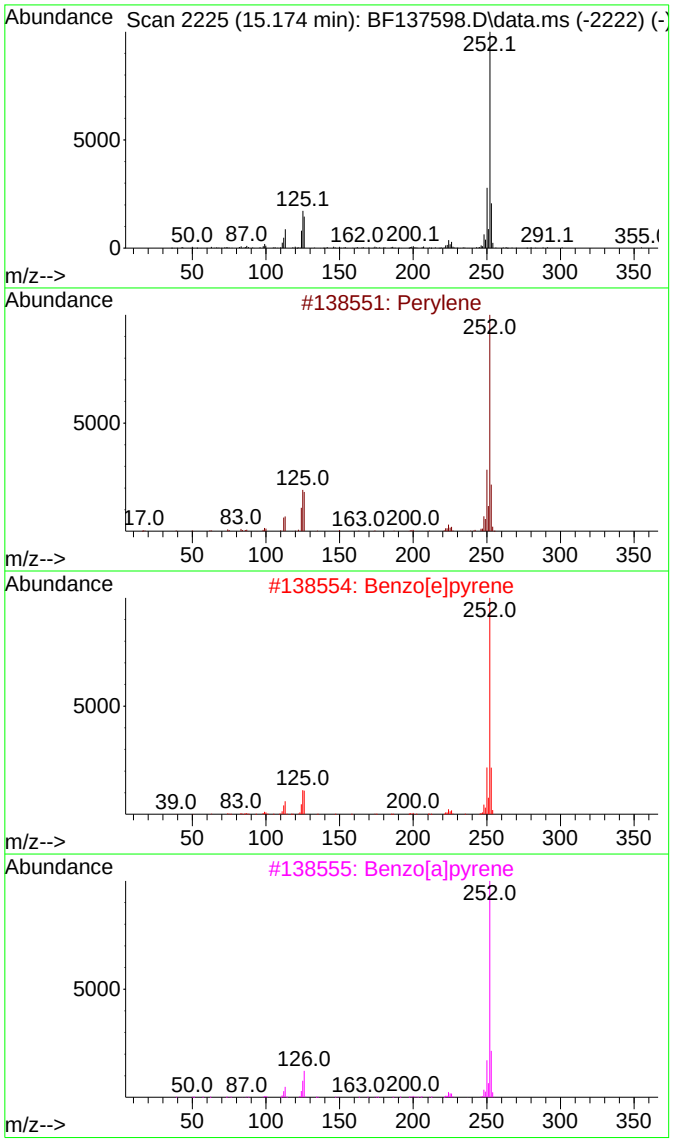
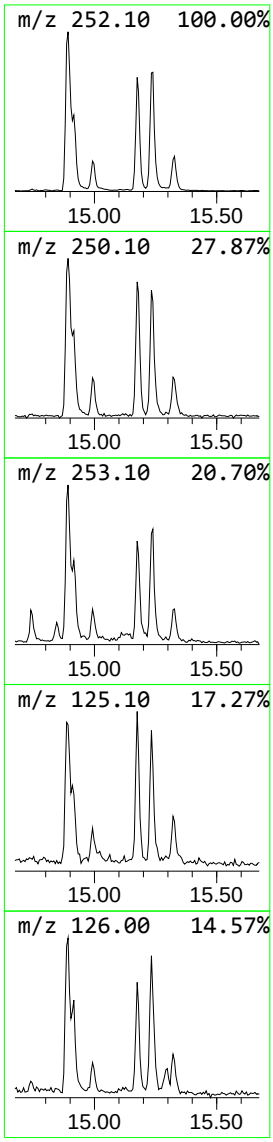
Peak Number 7 Perylene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.174	3.62 ng	170176	Perylene-d12	15.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	99
2	Benzo[e]pyrene	252	C20H12	000192-97-2	98
3	Benzo[a]pyrene	252	C20H12	000050-32-8	96
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	89





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Data File : BF137598.D
Acq On : 14 Mar 2024 19:00
Operator : CG\JU
Sample : P1744-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-3488

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.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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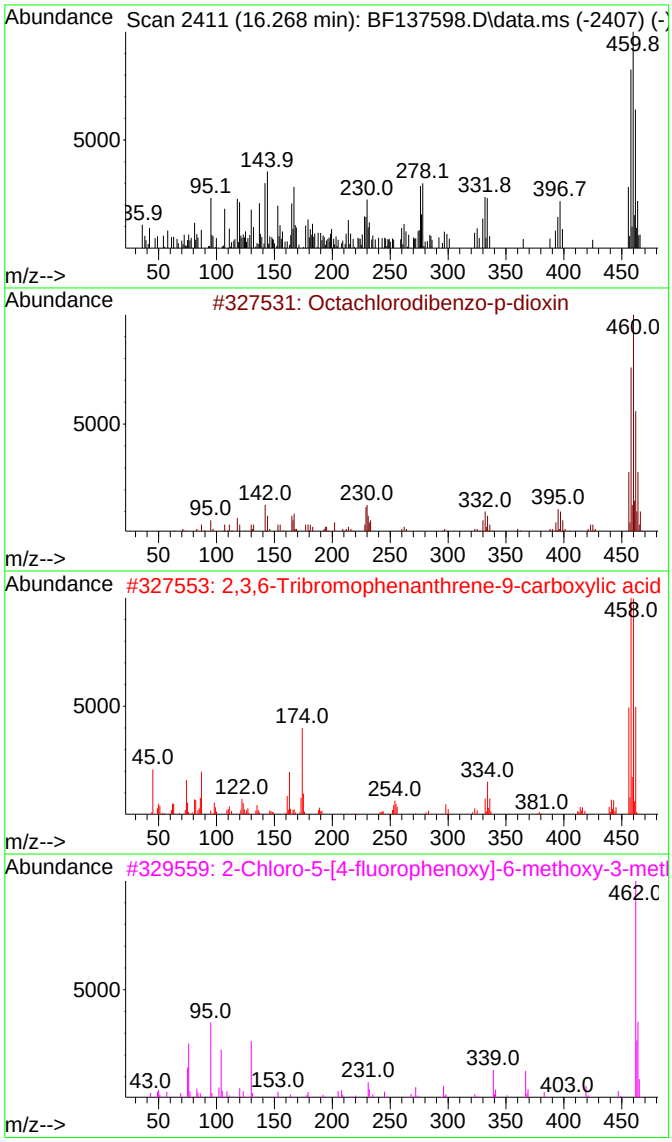
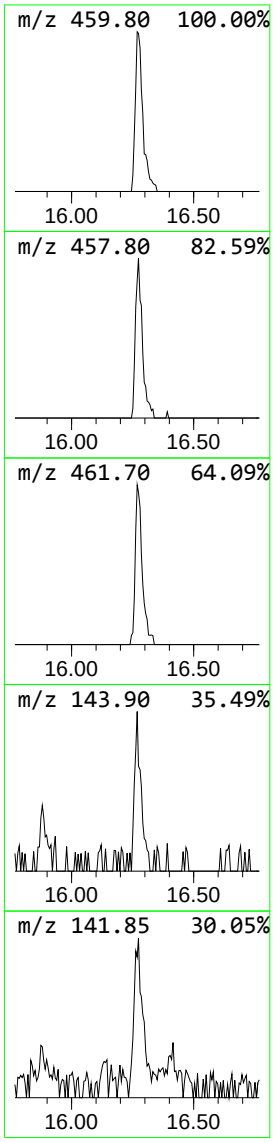
Peak Number 8 Octachlorodibenzo-p-dioxin Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.268	2.37 ng	111543	Perylene-d12	15.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octachlorodibenzo-p-dioxin	456	C12Cl8O2	003268-87-9	91
2	2,3,6-Tribromophenanthrene-9-car...	456	C15H7Br3O2	056988-60-4	35
3	2-Chloro-5-[4-fluorophenoxy]-6-m...	462	C25H16ClFN2O4	1000211-95-1	11
4	6-Ethyl-7-hydroxy-4-phenyl-2H-1-...	462	C21H13F7O4	1000462-90-8	10
5	N,N,N',N'-Tetra(trimethylsilyl)-...	460	C18H40N2S2Si4	135577-97-8	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031424\
Data File : BF137598.D
Acq On : 14 Mar 2024 19:00
Operator : CG\JU
Sample : P1744-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-3488

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.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
n-Hexadecanoic ...	11.775	5.1	ng	297139	4	11.239	1170180	20.0
4H-Cyclopenta[d...	11.851	2.2	ng	131089	4	11.239	1170180	20.0
Pyrene, 4-methyl-	13.204	2.0	ng	119485	5	13.874	1190840	20.0
3-Eicosene, (E)-	13.739	4.5	ng	270010	5	13.874	1190840	20.0
1-Heptacosanol	14.380	2.6	ng	157257	5	13.874	1190840	20.0
(3E,7E)-4,8,12-...	14.716	2.5	ng	117004	6	15.292	939842	20.0
Perylene	15.174	3.6	ng	170176	6	15.292	939842	20.0
Octachlorodiben...	16.268	2.4	ng	111543	6	15.292	939842	20.0