LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112524\
Data File : BF140609.D
Acq On : 25 Nov 2024 18:07
Operator : RC/JU
Sample : P4860-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP-01

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-BF112124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140609.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.087	504	509	518	rVB	21181	31645	1.74%	0.255%
2	5.492	573	578	594	rBV	952643	1322198	72.86%	10.637%
3	6.504	744	750	771	rBV	1066743	1437303	79.21%	11.563%
4	6.869	807	812	819	rBV	313561	379664	20.92%	3.054%
5	7.428	902	907	918	rBV	688756	908768	50.08%	7.311%
6	8.151	1024	1030	1044	rBV	361539	478807	26.39%	3.852%
7	9.222	1207	1212	1222	rBV	1417930	1786621	98.46%	14.373%
8	9.904	1323	1328	1340	rBV	427158	546386	30.11%	4.396%
9	10.616	1444	1449	1457	rBV	99351	126824	6.99%	1.020%
10	10.698	1457	1463	1477	rVV	698988	969983	53.45%	7.804%
11	10.810	1477	1482	1489	rVB4	9027	19825	1.09%	0.159%
12	11.392	1576	1581	1589	rBV	438315	601408	33.14%	4.838%
13	11.916	1665	1670	1682	rBV	134906	228074	12.57%	1.835%
14	12.339	1737	1742	1746	rBV2	57119	74573	4.11%	0.600%
15	12.615	1784	1789	1791	rBV	35097	53959	2.97%	0.434%
16	12.645	1791	1794	1800	rVV	72874	103878	5.72%	0.836%
17	12.704	1800	1804	1810	rVB	19837	34090	1.88%	0.274%
18	12.839	1823	1827	1834	rVB2	22493	31841	1.75%	0.256%
19	12.980	1845	1851	1856	rBV	1433570	1814641	100.00%	14.599%
20	13.115	1869	1874	1879	rBV	127615	157157	8.66%	1.264%
21	13.545	1942	1947	1952	rBV	24399	32950	1.82%	0.265%
22	13.874	1998	2003	2005	rBV	29293	45690	2.52%	0.368%
23	14.045	2027	2032	2043	rVB	300603	432045	23.81%	3.476%
24	14.192	2053	2057	2062	rVB	28407	36959	2.04%	0.297%
25	14.504	2106	2110	2115	rBV	31032	41788	2.30%	0.336%
26	14.815	2159	2163	2169	rVB	24351	33859	1.87%	0.272%
27	14.892	2173	2176	2183	rVB	17829	24382	1.34%	0.196%
28	15.157	2216	2221	2226	rBV	29850	43815	2.41%	0.352%
29	15.539	2280	2286	2297	rBV	221846	372267	20.51%	2.995%
30	15.986	2358	2362	2368	rVB2	14658	23319	1.29%	0.188%
31	16.286	2405	2413	2433	rVB2	22236	111314	6.13%	0.896%
32	16.445	2434	2440	2445	rBV2	58154	105767	5.83%	0.851%
33	17.656	2641	2646	2650	rBV6	8622	18230	1.00%	0.147%

Sum of corrected areas: 12430030

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112524\
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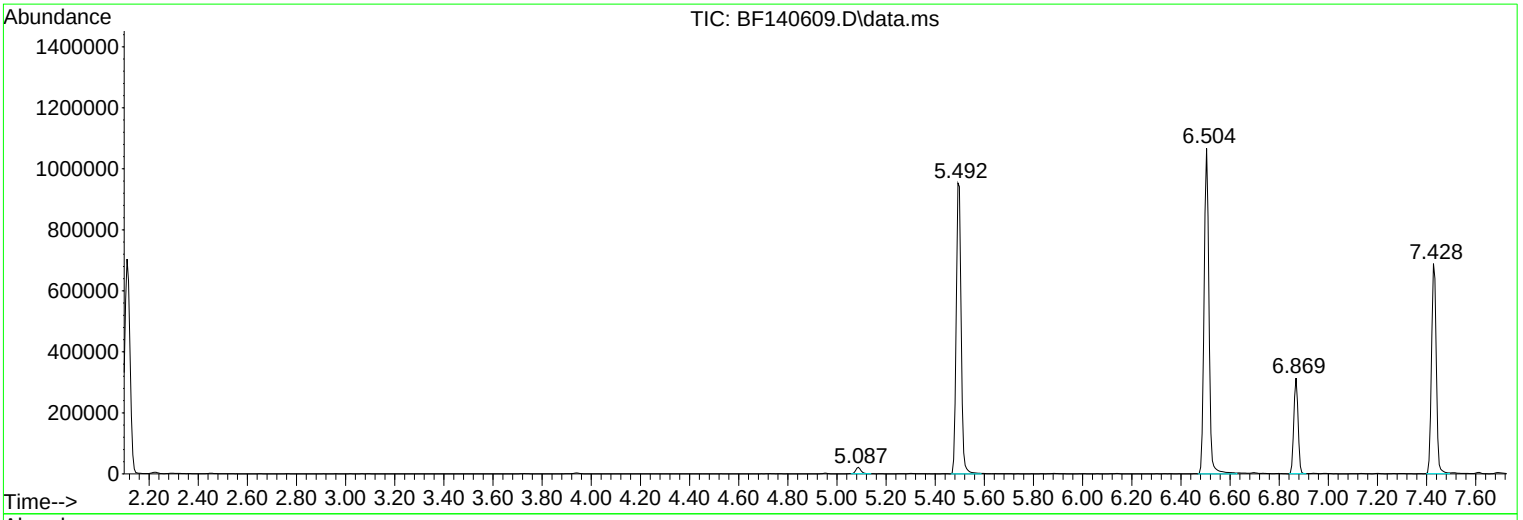
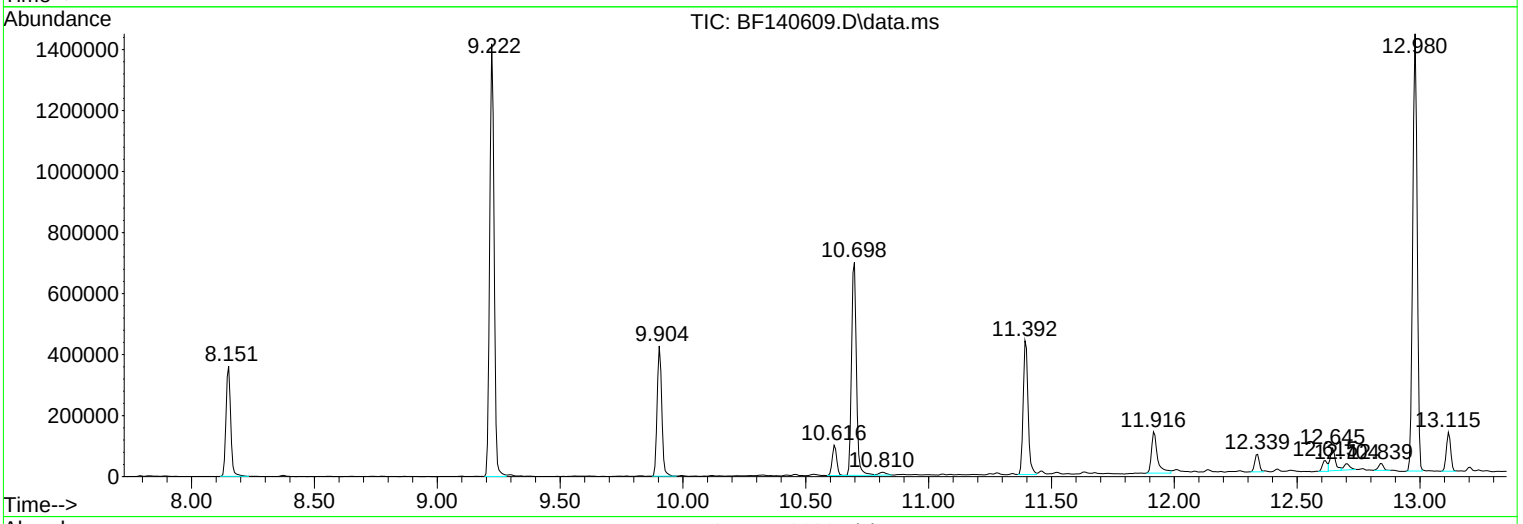
Misc :
ALS Vial : 7 Sample Multiplier: 1

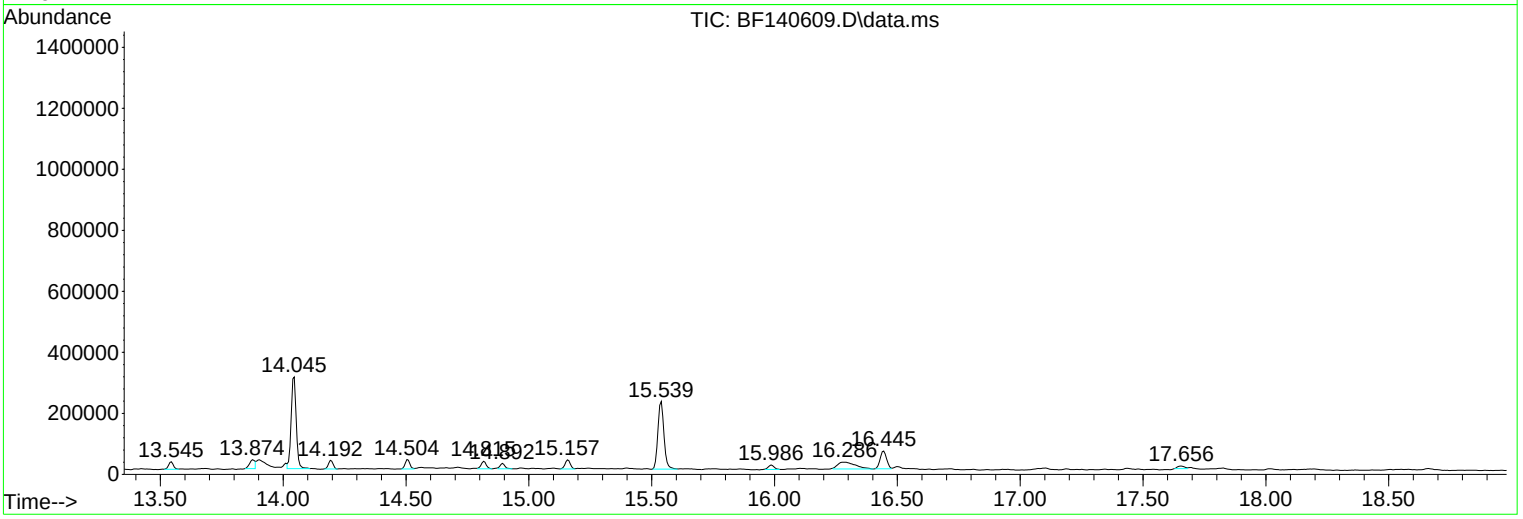
Instrument :
BNA_F
ClientSampleId :
DUP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.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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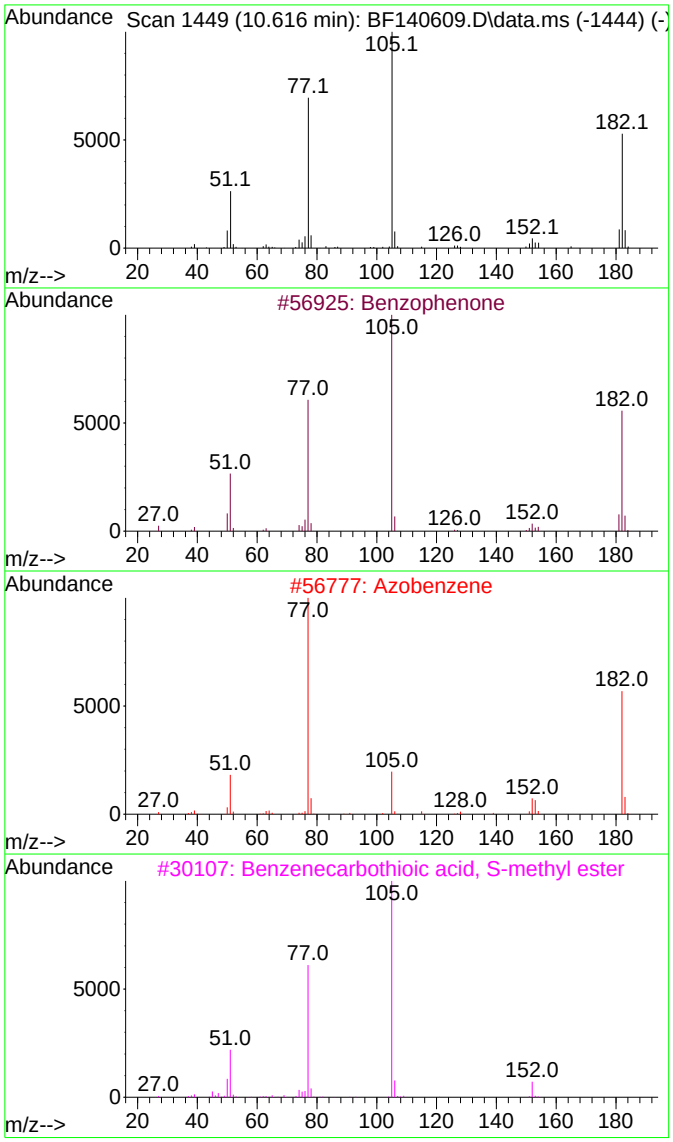
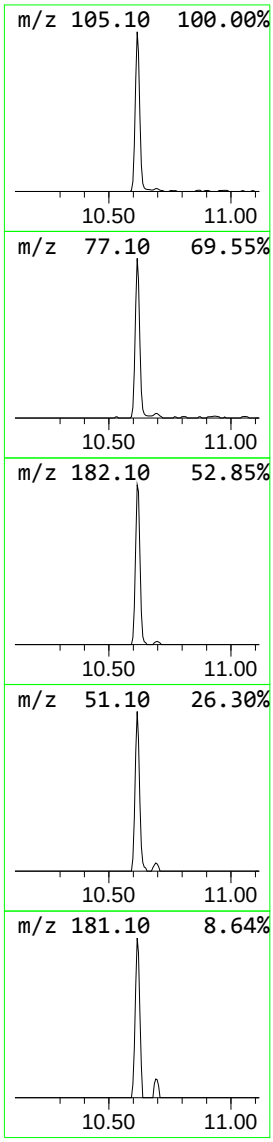
Peak Number 1 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.616	4.64 ng	126824	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	64
3	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
4	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	49
5	Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	49





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ClientSampleId :
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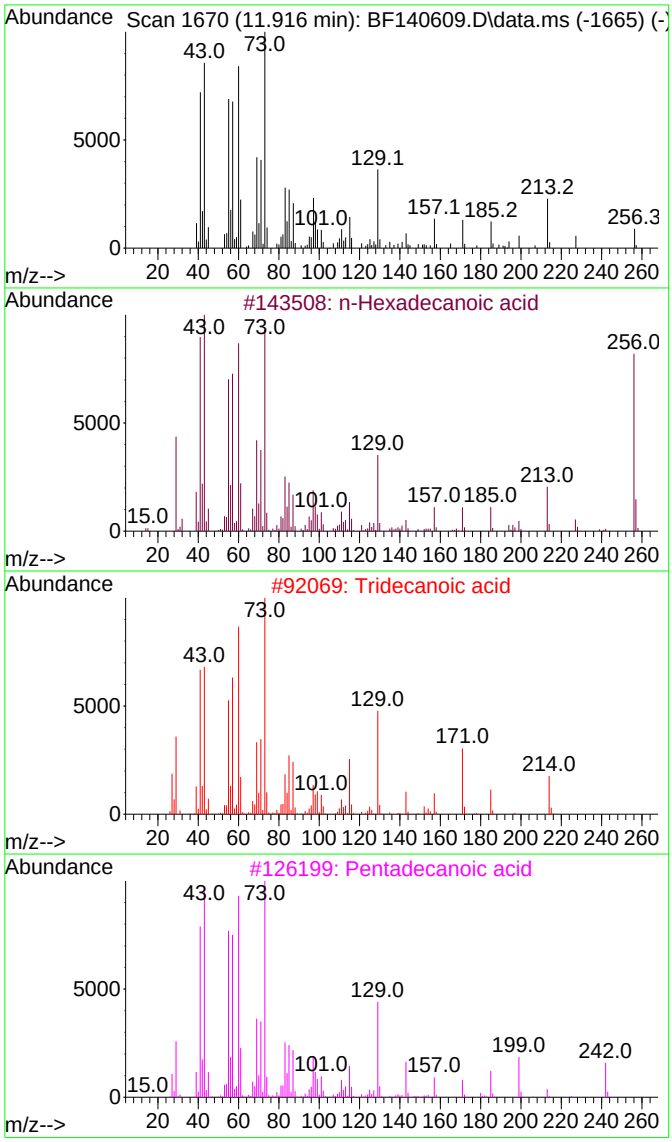
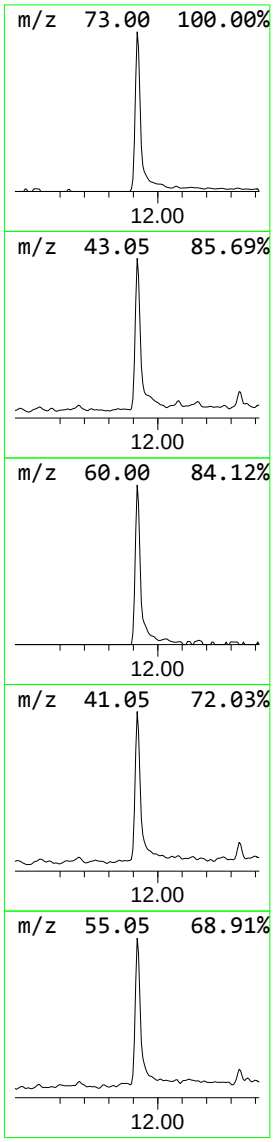
Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	7.58 ng	228074	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.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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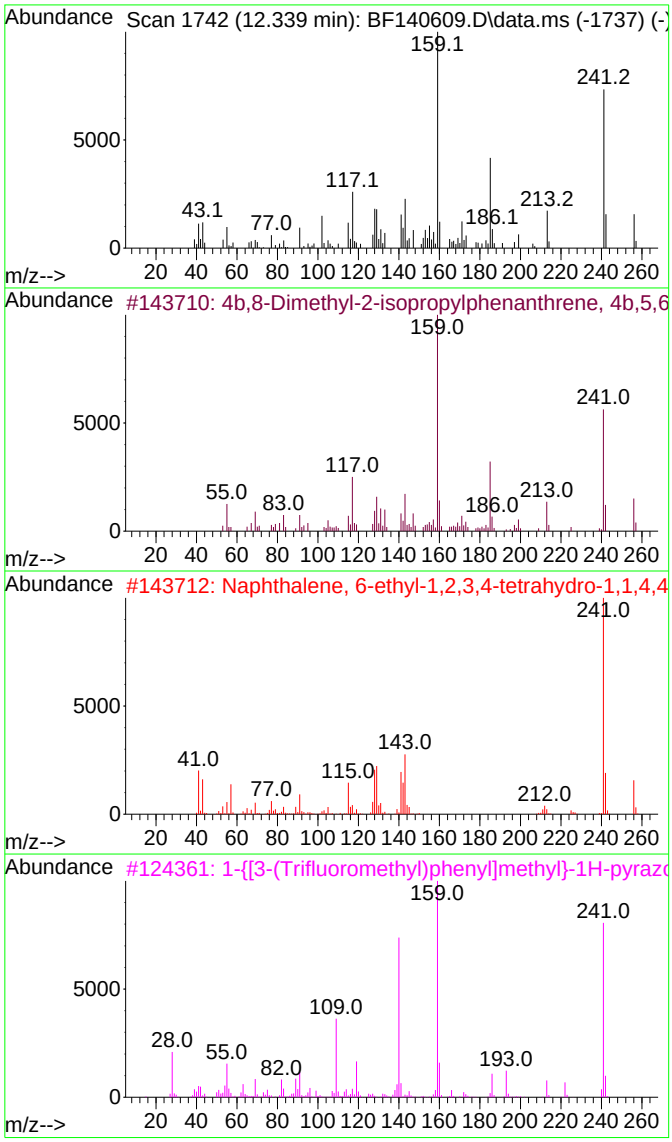
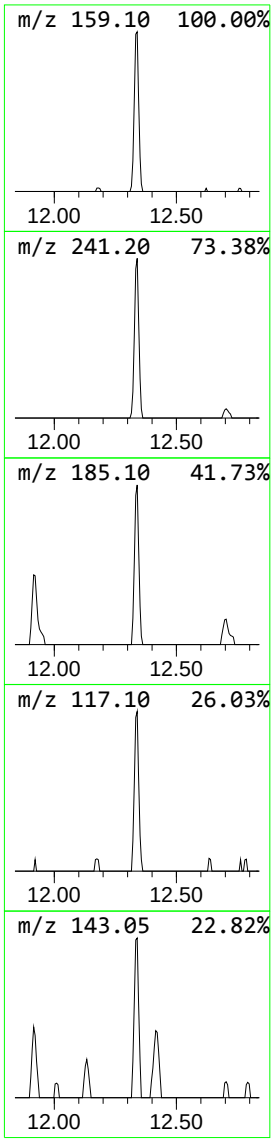
Peak Number 3 4b,8-Dimethyl-2-isopropylph... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.339	2.48 ng	74573	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4b,8-Dimethyl-2-isopropylphenant...	256	C19H28	1000197-14-1	95
2	Naphthalene, 6-ethyl-1,2,3,4-tet...	256	C19H28	301643-35-6	52
3	1-{[3-(Trifluoromethyl)phenyl]me...	241	C11H10F3N3	1002033-51-3	52
4	3,4-Dihydro-3,3-dimethyl-1,9(2H,...	241	C15H15NO2	1010212-95-2	45
5	s-Indacen-1(2H)-one, 3,5,6,7-tet...	256	C18H24O	038754-94-8	30





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ClientSampleId :
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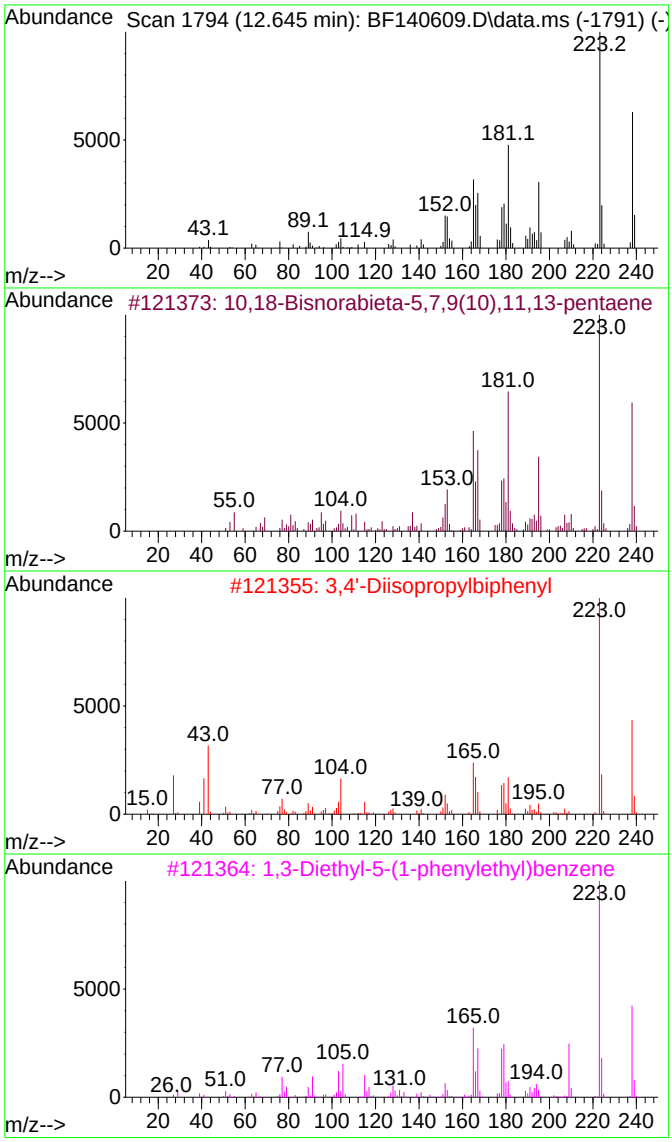
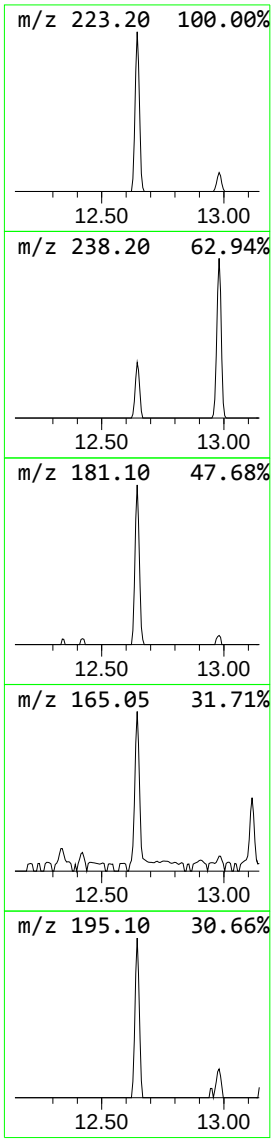
Peak Number 4 10,18-Bisnorabieta-5,7,9(10... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	3.45 ng	103878	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10,18-Bisnorabieta-5,7,9(10),11,...	238	C18H22	006566-19-4	99
2	3,4'-Diisopropylbiphenyl	238	C18H22	061434-46-6	90
3	1,3-Diethyl-5-(1-phenylethyl)ben...	238	C18H22	1000482-32-6	89
4	3-(N,N-Diethylamino)carbazole	238	C16H18N2	054994-31-9	64
5	4,4'-Diisopropylbiphenyl	238	C18H22	018970-30-4	53





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Sample : P4860-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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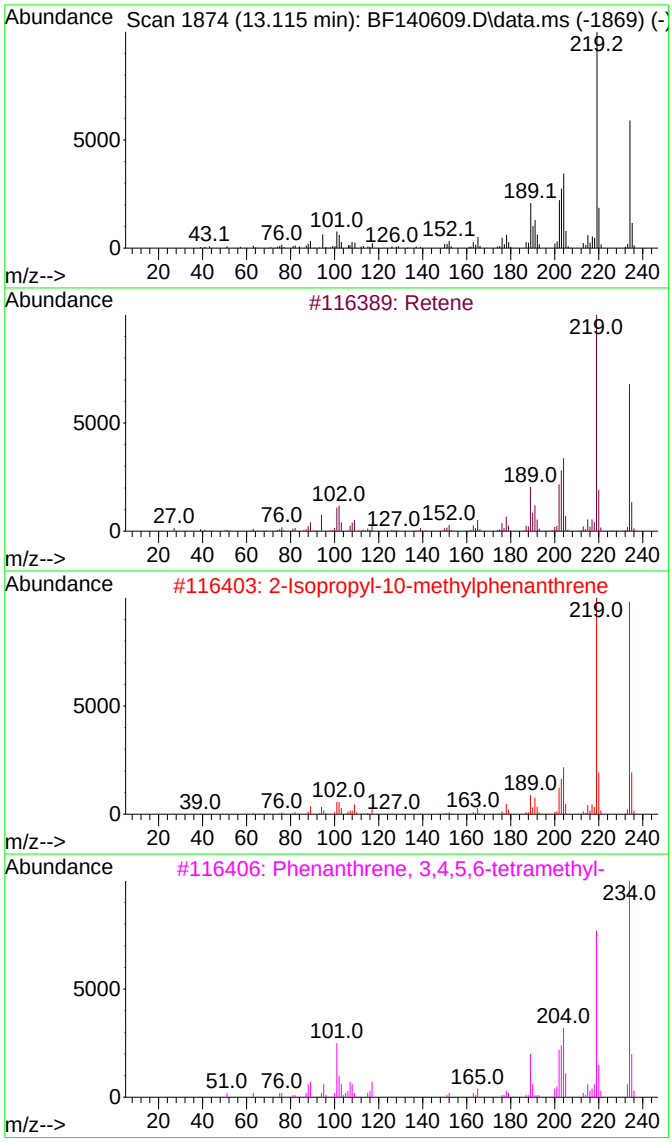
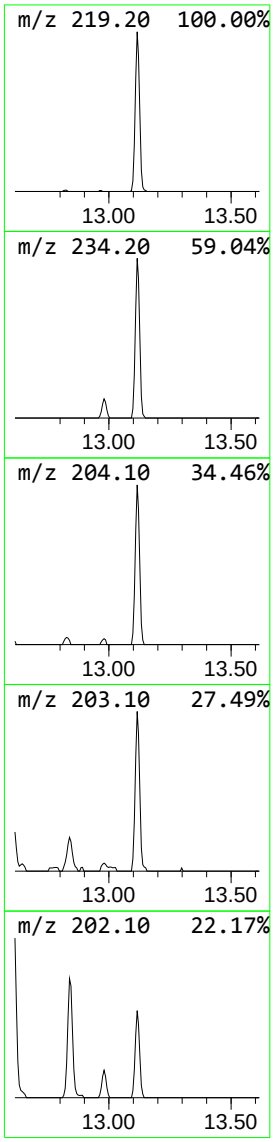
Peak Number 5 Retene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.116	7.28 ng	157157	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Retene	234	C18H18	000483-65-8	98
2	2-Isopropyl-10-methylphenanthrene	234	C18H18	066552-97-4	95
3	Phenanthrene, 3,4,5,6-tetramethyl-	234	C18H18	007343-06-8	76
4	Phenanthrene, 2,4,5,7-tetramethyl-	234	C18H18	007396-38-5	62
5	1-(10-Methylanthracen-9-yl)ethanone	234	C17H14O	036778-18-4	58





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TIC Library : C:\Database\NIST20.L
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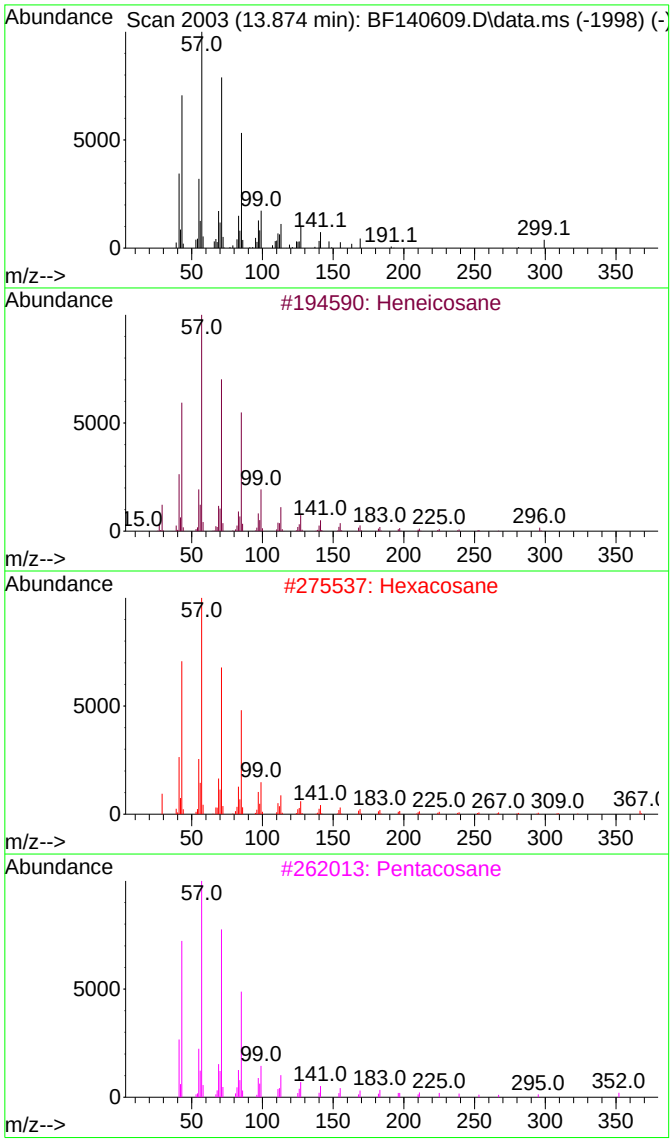
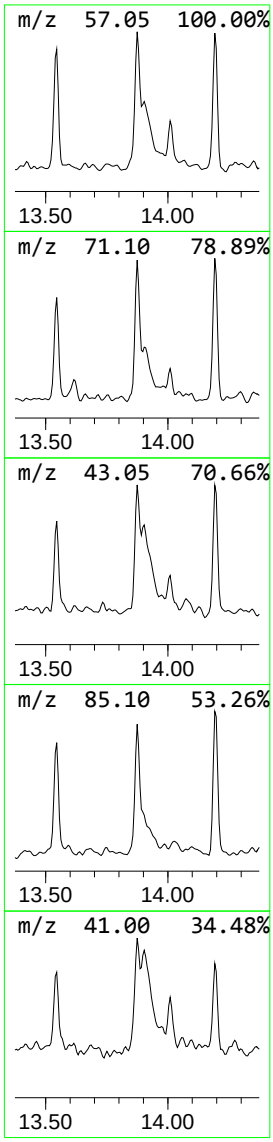
Peak Number 6 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	2.12 ng	45690	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Pentacosane	352	C25H52	000629-99-2	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Eicosane	282	C20H42	000112-95-8	91





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BNA_F
ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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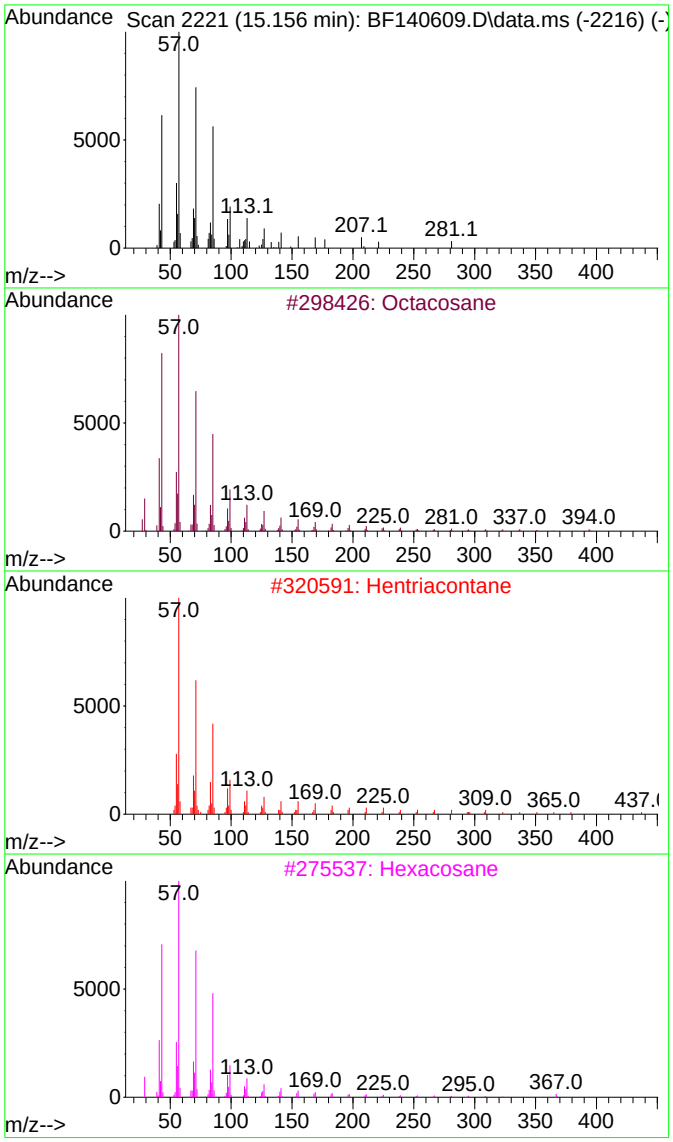
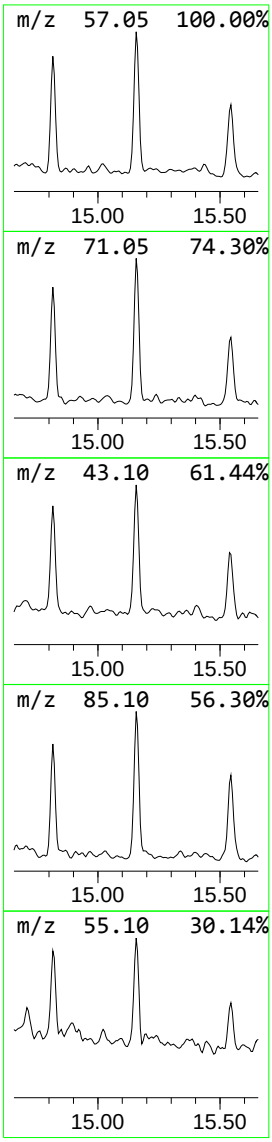
Peak Number 7 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.156	2.35 ng	43815	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hentriacontane	437	C31H64	000630-04-6	91
3	Hexacosane	366	C26H54	000630-01-3	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Heptacosane	380	C27H56	000593-49-7	87





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BNA_F
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TIC Library : C:\Database\NIST20.L
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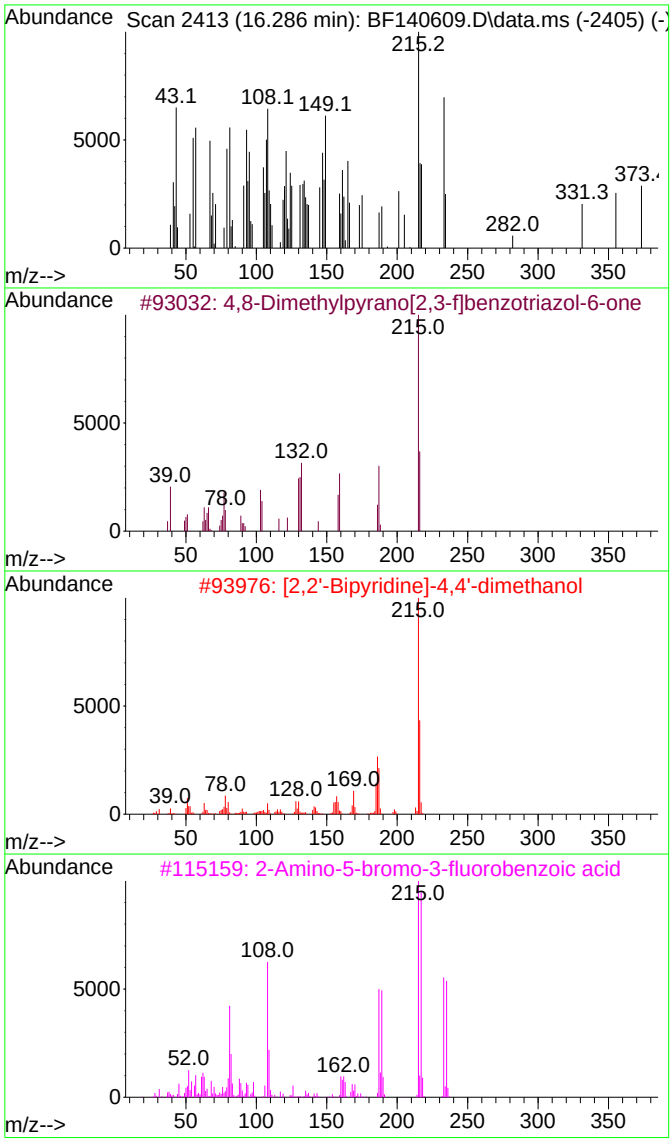
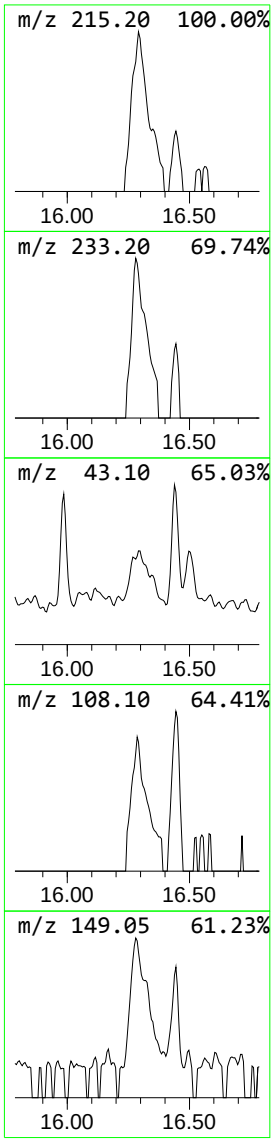
Peak Number 8 unknown16.286 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.286	5.98 ng	111314	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,8-Dimethylpyrano[2,3-f]benzotr...	215	C11H9N3O2	129503-12-4	14
2	[2,2'-Bipyridine]-4,4'-dimethanol	216	C12H12N2O2	109073-77-0	12
3	2-Amino-5-bromo-3-fluorobenzoic ...	233	C7H5BrFNO2	874784-14-2	12
4	4-Methyl-2H,3H,3aH-pyrrolo[1,2-a...	216	C12H12N2O2	1000387-53-2	12
5	2-Cyclohexen-3-ol-1-one, 2-benzoyl-	216	C13H12O3	061834-43-3	10





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Operator : RC/JU
Sample : P4860-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

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ClientSampleId :
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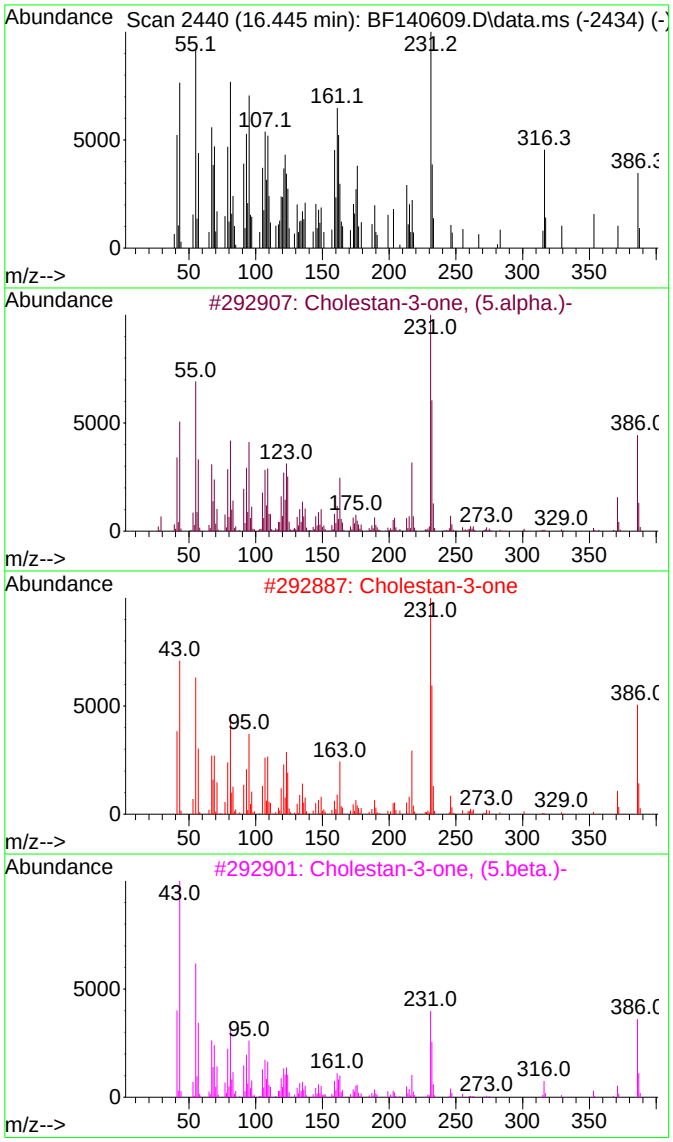
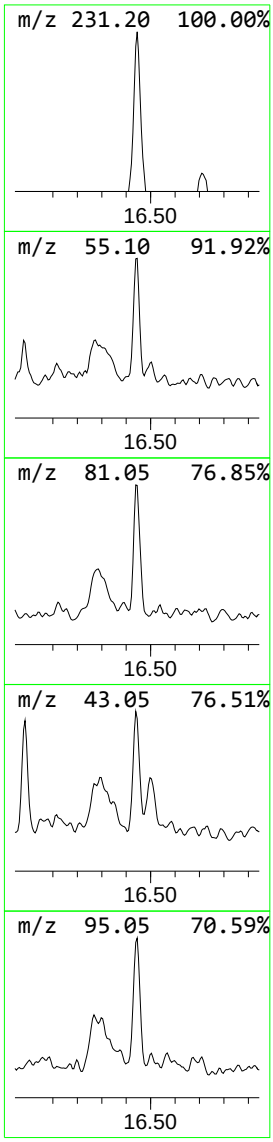
Peak Number 9 Cholestan-3-one, (5.alpha.)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.445	5.68 ng	105767	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholestan-3-one, (5.alpha.)-	386	C27H46O	000566-88-1	91
2	Cholestan-3-one	386	C27H46O	015600-08-5	91
3	Cholestan-3-one, (5.beta.)-	386	C27H46O	000601-53-6	86
4	Cholestane, 14-methyl-, (5.alpha.)-	386	C28H50	054482-34-7	30
5	Cholestane, 14-methyl-	386	C28H50	052474-84-7	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112524\
Data File : BF140609.D
Acq On : 25 Nov 2024 18:07
Operator : RC/JU
Sample : P4860-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.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
Benzophenone	10.616	4.6	ng	126824	3	9.904	546386	20.0
n-Hexadecanoic ...	11.916	7.6	ng	228074	4	11.392	601408	20.0
4b,8-Dimethyl-2...	12.339	2.5	ng	74573	4	11.392	601408	20.0
10,18-Bisnorabi...	12.645	3.5	ng	103878	4	11.392	601408	20.0
Retene	13.116	7.3	ng	157157	5	14.045	432045	20.0
Heneicosane	13.874	2.1	ng	45690	5	14.045	432045	20.0
Octacosane	15.156	2.4	ng	43815	6	15.539	372267	20.0
unknown16.286	16.286	6.0	ng	111314	6	15.539	372267	20.0
Cholestan-3-one...	16.445	5.7	ng	105767	6	15.539	372267	20.0