LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071023\
Data File : BF134194.D
Acq On : 10 Jul 2023 19:31
Operator : CG\JU
Sample : 03507-04 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CP-2

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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134194.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.069	503	507	518	rVB	32323	37752	4.33%	0.358%
2	5.469	572	575	594	rBV	854907	841256	96.55%	7.986%
3	6.475	743	746	756	rBV	939584	836544	96.01%	7.941%
4	6.840	805	808	817	rBV	830755	741106	85.06%	7.035%
5	7.398	900	903	912	rBV	555170	502088	57.62%	4.766%
6	8.122	1022	1026	1029	rBV	1151165	871316	100.00%	8.271%
7	9.198	1205	1209	1212	rBV	996648	815424	93.59%	7.741%
8	9.275	1219	1222	1225	rVB	28854	24011	2.76%	0.228%
9	9.534	1264	1266	1269	rBV3	19967	20666	2.37%	0.196%
10	9.598	1275	1277	1283	rVB3	22488	25080	2.88%	0.238%
11	9.739	1298	1301	1306	rBV	55034	51468	5.91%	0.489%
12	9.810	1311	1313	1317	rVB	28035	22519	2.58%	0.214%
13	9.881	1321	1325	1328	rBV	960346	777509	89.23%	7.381%
14	10.081	1355	1359	1364	rBV	45719	58940	6.76%	0.560%
15	10.122	1364	1366	1372	rVB6	13410	18599	2.13%	0.177%
16	10.310	1396	1398	1400	rVB	29131	20725	2.38%	0.197%
17	10.428	1415	1418	1425	rBV2	13822	20344	2.33%	0.193%
18	10.533	1432	1436	1441	rVB3	13420	19525	2.24%	0.185%
19	10.592	1443	1446	1454	rVV	79539	88172	10.12%	0.837%
20	10.669	1456	1459	1470	rVB	401833	388831	44.63%	3.691%
21	10.786	1476	1479	1484	rVB2	29896	47498	5.45%	0.451%
22	11.375	1575	1579	1582	rBV	829412	724977	83.20%	6.882%
23	11.398	1582	1583	1587	rVV	78964	48882	5.61%	0.464%
24	11.451	1589	1592	1595	rVV	69213	58162	6.68%	0.552%
25	11.880	1663	1665	1666	rBV	24646	20705	2.38%	0.197%
26	11.904	1666	1669	1674	rVB2	111837	117785	13.52%	1.118%
27	11.992	1680	1684	1687	rBV2	44204	54428	6.25%	0.517%
28	12.175	1713	1715	1718	rBV2	19891	24841	2.85%	0.236%
29	12.304	1735	1737	1742	rBV4	29639	37972	4.36%	0.360%
30	12.357	1744	1746	1748	rBV3	25363	29270	3.36%	0.278%
31	12.433	1756	1759	1761	rBV	52929	53798	6.17%	0.511%
32	12.527	1772	1775	1777	rBV3	30477	45355	5.21%	0.431%
33	12.598	1784	1787	1789	rBV	98071	98123	11.26%	0.931%
34	12.645	1792	1795	1799	rVB4	80285	114856	13.18%	1.090%
35	12.698	1801	1804	1807	rVB2	82986	75204	8.63%	0.714%
36	12.751	1811	1813	1815	rBV	51306	48763	5.60%	0.463%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071023\
Data File : BF134194.D
Acq On : 10 Jul 2023 19:31
Operator : CG\JU
Sample : 03507-04 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CP-2

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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.827	1823	1826	1833	rBV	250689	283032	32.48%	2.687%
38	12.969	1847	1850	1857	rBV	871105	791211	90.81%	7.511%
39	13.151	1879	1881	1885	rVB3	138930	158146	18.15%	1.501%
40	13.463	1931	1934	1938	rBV5	110448	170407	19.56%	1.618%
41	14.039	2029	2032	2035	rBV	555270	516240	59.25%	4.901%
42	16.280	2410	2413	2420	rVB	525518	832752	95.57%	7.905%

Sum of corrected areas: 10534282

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Operator : CG\JU
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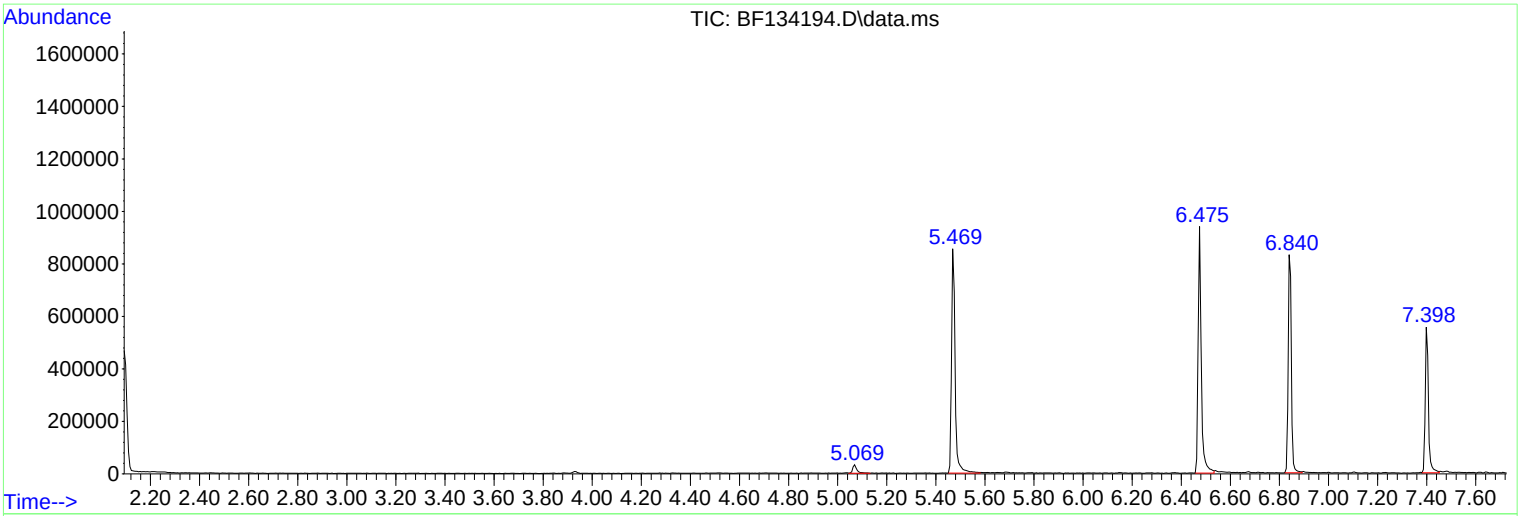
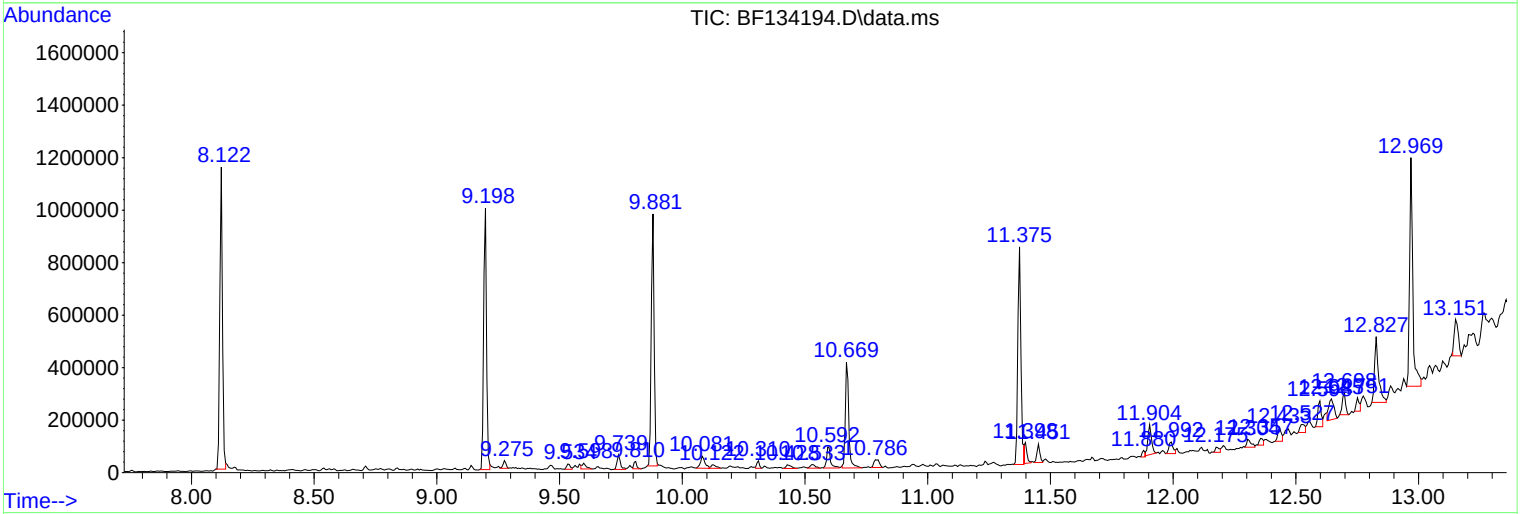
Misc :
ALS Vial : 13 Sample Multiplier: 1

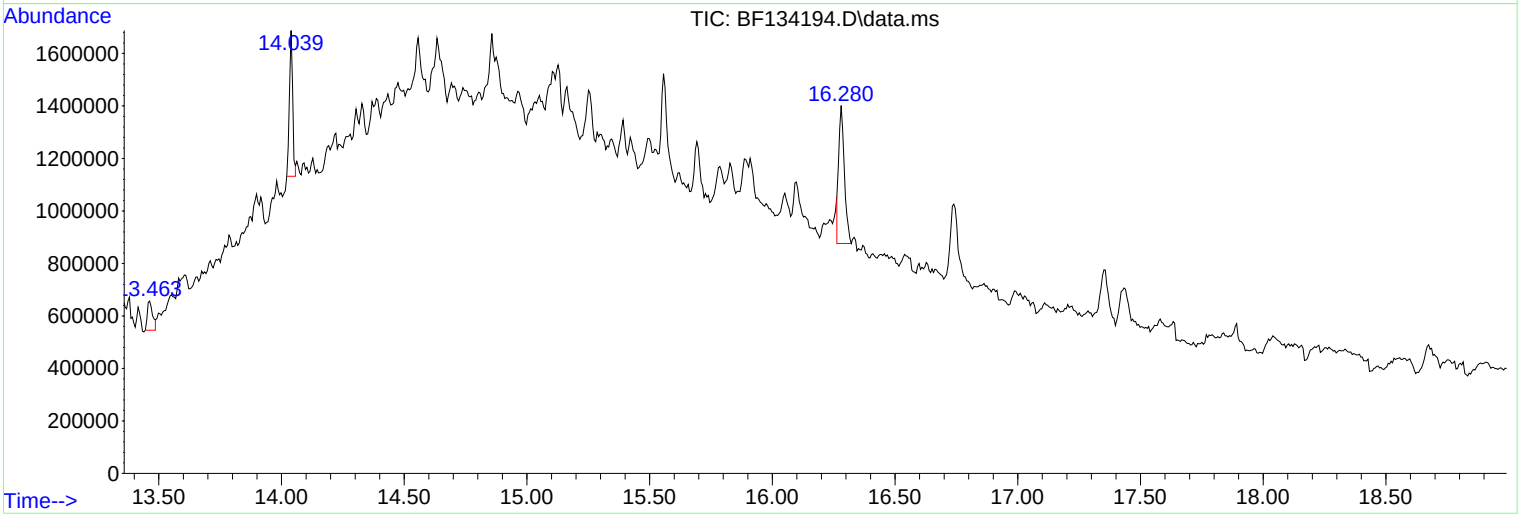
Instrument :
BNA_F
ClientSampleId :
CP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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\BF071023\
Data File : BF134194.D
Acq On : 10 Jul 2023 19:31
Operator : CG\JU
Sample : 03507-04 2X
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BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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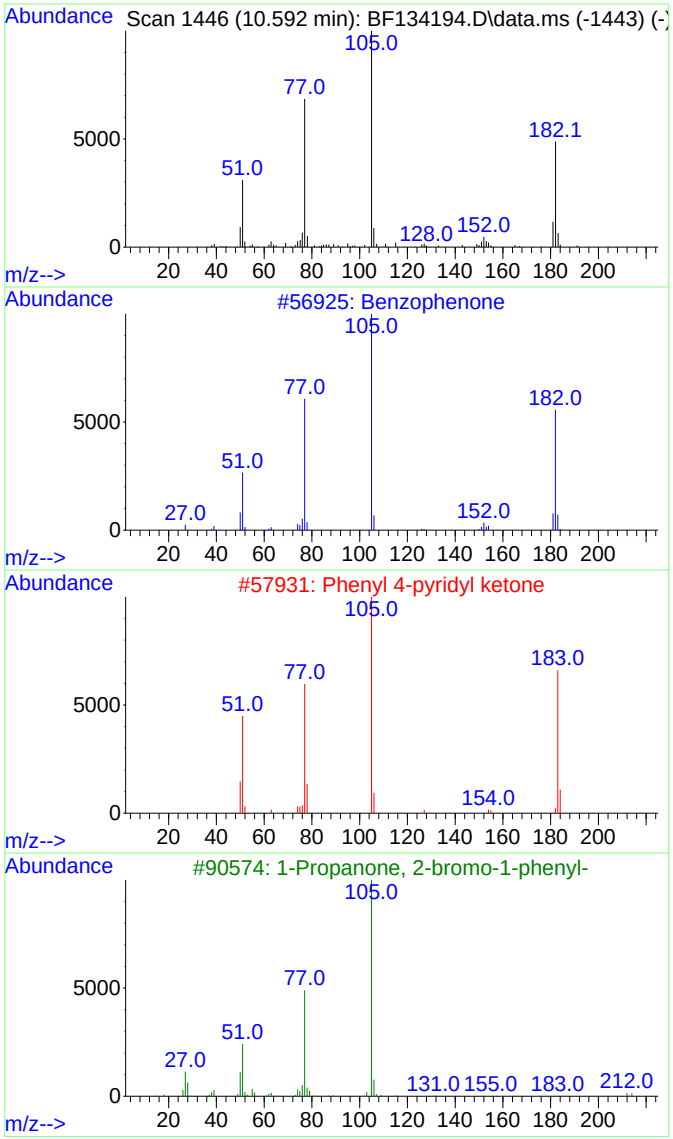
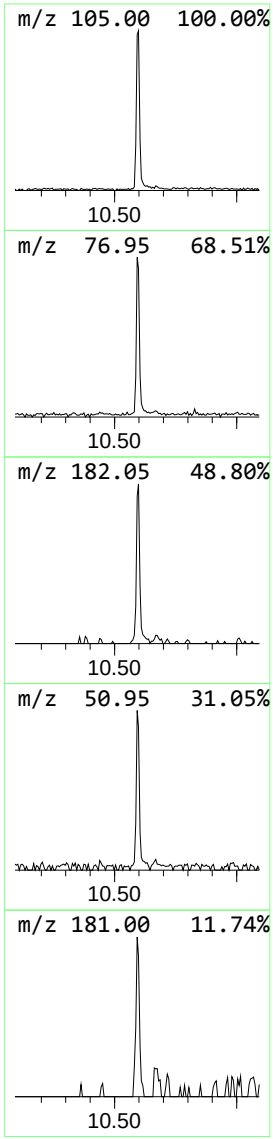
Peak Number 1 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.592	2.27 ng	88172	Acenaphthene-d10	9.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	53
3	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4	Azobenzene	182	C12H10N2	000103-33-3	47
5	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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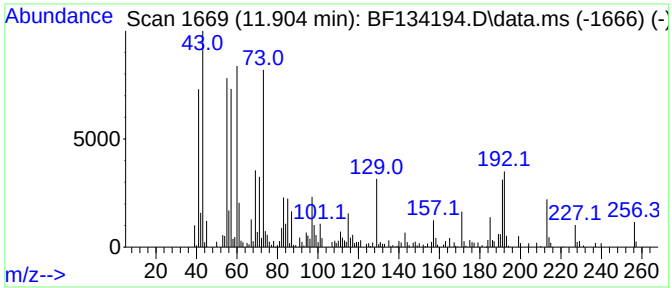
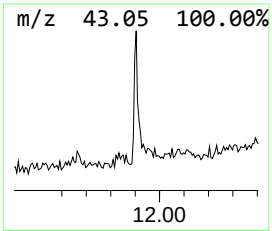
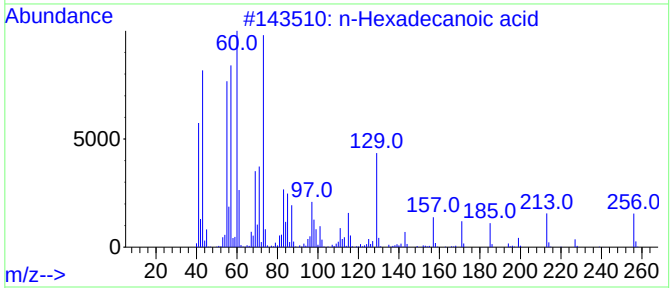
Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

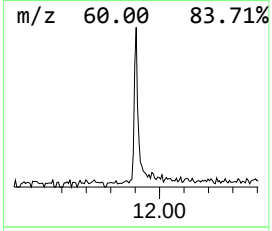
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	3.25 ng	117785	Phenanthrene-d10	11.374

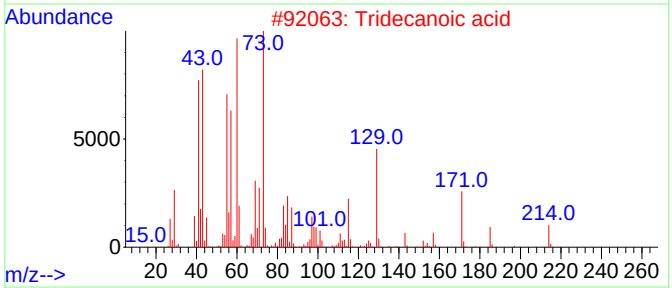
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Undecanoic acid	186	C11H22O2	000112-37-8	53

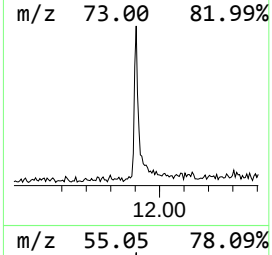


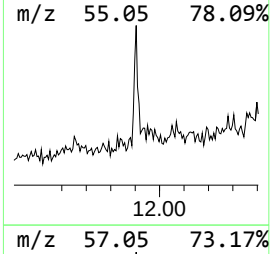


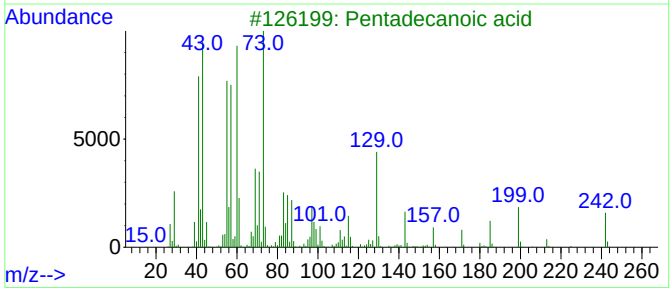


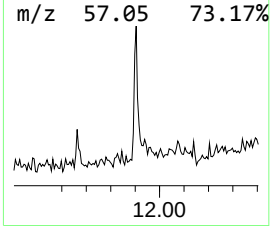












Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071023\
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Operator : CG\JU
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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

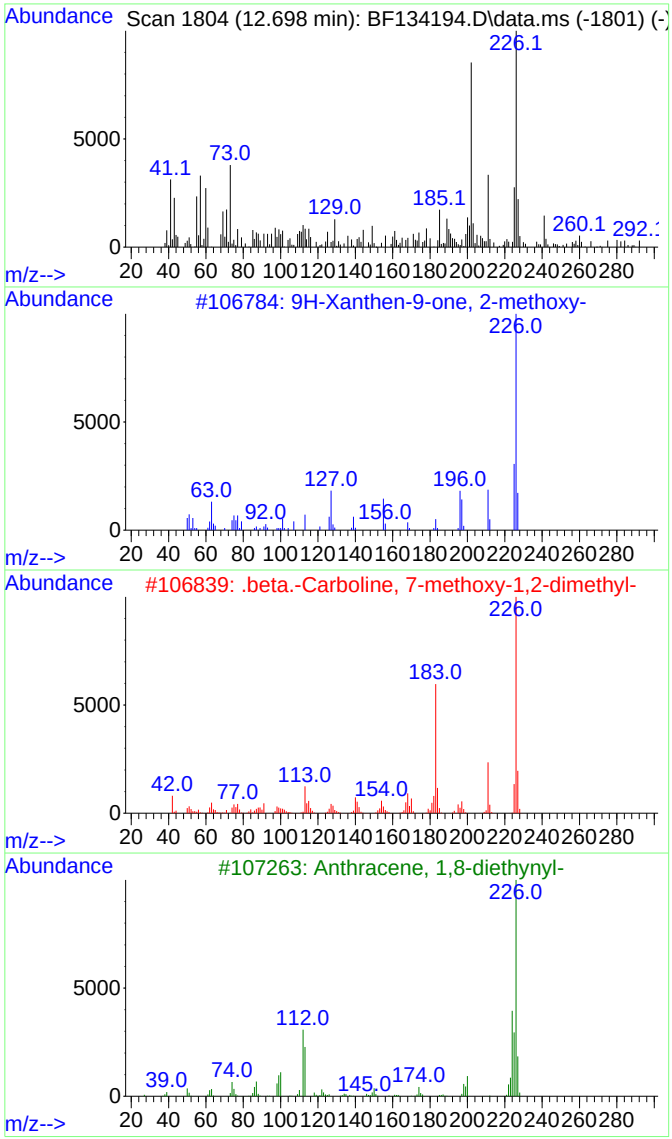
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

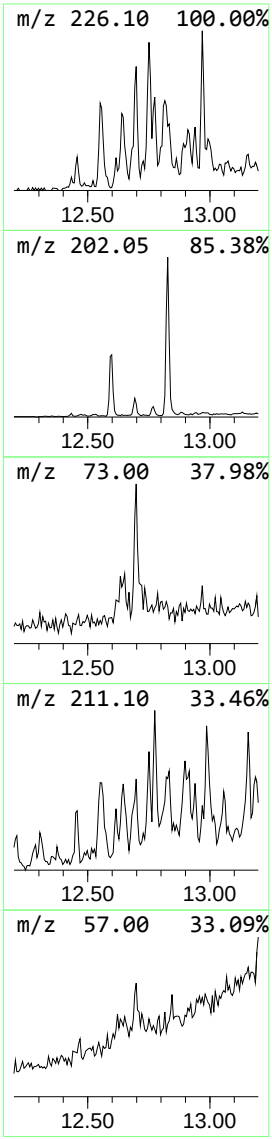
****

Peak Number 3 unknown12.698 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.698	2.07 ng	75204	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9H-Xanthen-9-one, 2-methoxy-	226	C14H10O3	001214-20-6	38
2	.beta.-Carboline, 7-methoxy-1,2-...	226	C14H14N2O	006519-18-2	38
3	Anthracene, 1,8-diethynyl-	226	C18H10	078053-58-4	38
4	5(10H)-Pyrido[3,4-b]quinolone, 7...	226	C13H10N2O2	1000256-99-5	35
5	1,3-Diamino-5,6-dihydro-7-methyl...	226	C13H14N4	037436-37-6	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071023\
Data File : BF134194.D
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Sample : 03507-04 2X
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Instrument :
BNA_F
ClientSampleId :
CP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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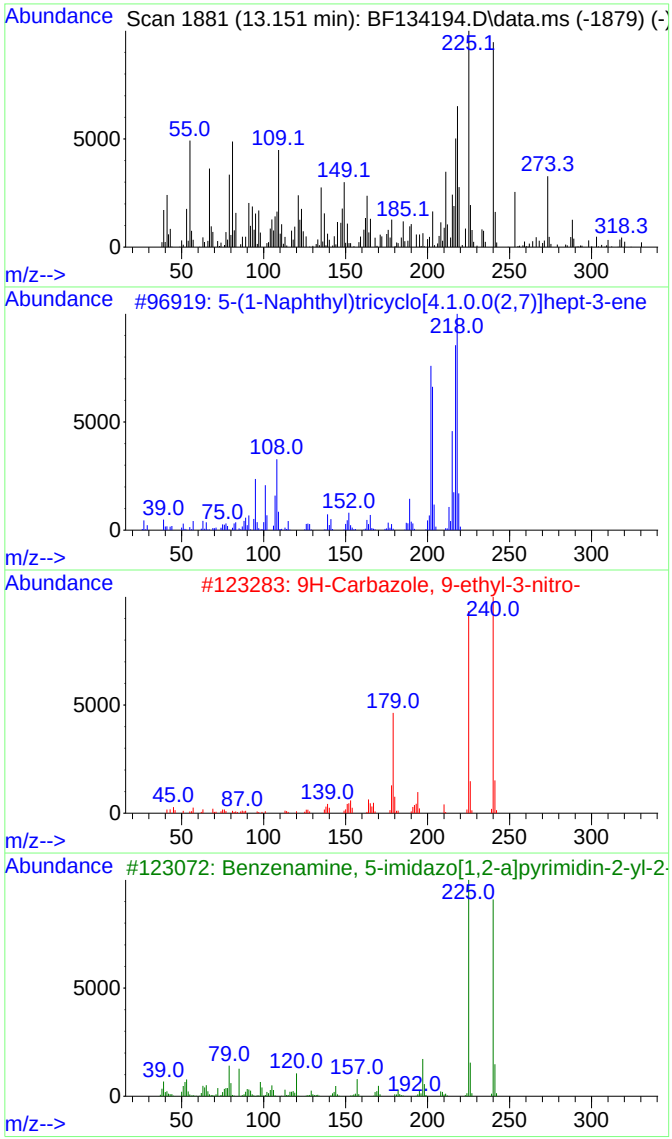
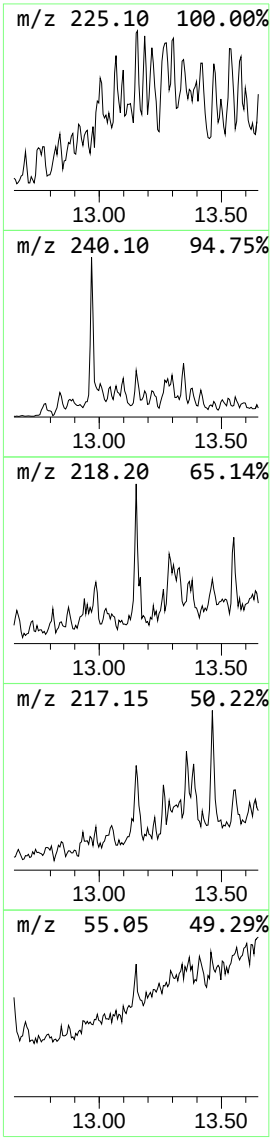
Peak Number 4 unknown13.151 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.151	6.13 ng	158146	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-(1-Naphthyl)tricyclo[4.1.0.0(2...	218	C17H14	107729-05-5	45
2	9H-Carbazole, 9-ethyl-3-nitro-	240	C14H12N2O2	000086-20-4	41
3	Benzenamine, 5-imidazo[1,2-a]pyr...	240	C13H12N4O	1010337-85-8	38
4	5-Amino-1-methyl-3-(methylsulfan...	240	C9H16N4SSi	1000474-43-3	38
5	Disulfide, diphenyl	218	C12H10S2	000882-33-7	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071023\
Data File : BF134194.D
Acq On : 10 Jul 2023 19:31
Operator : CG\JU
Sample : 03507-04 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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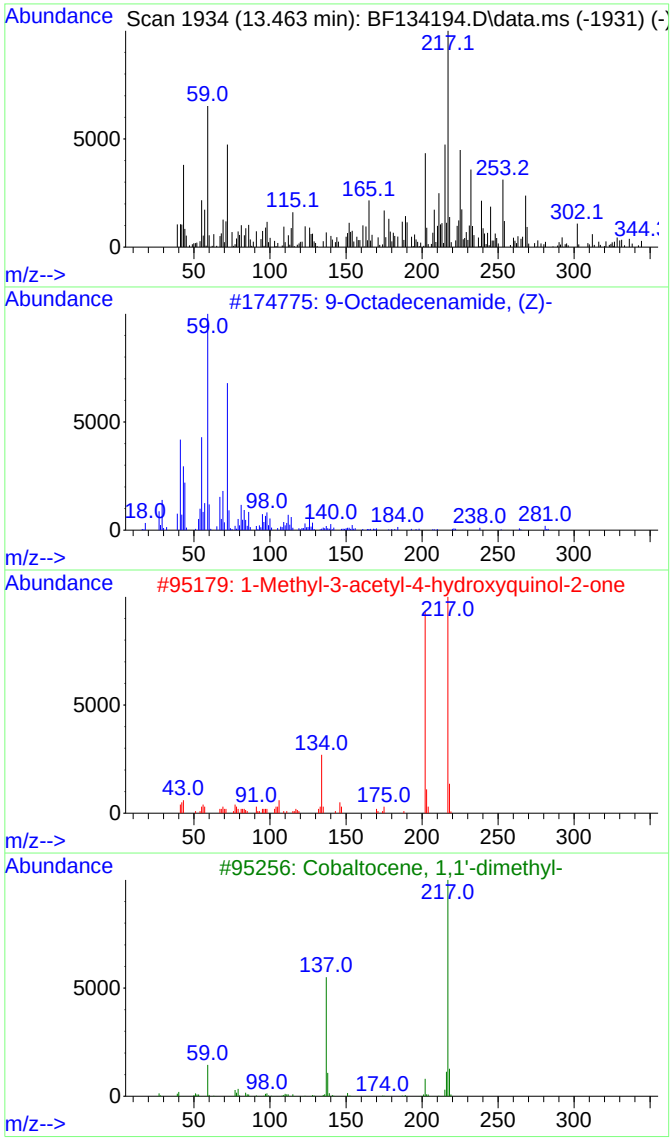
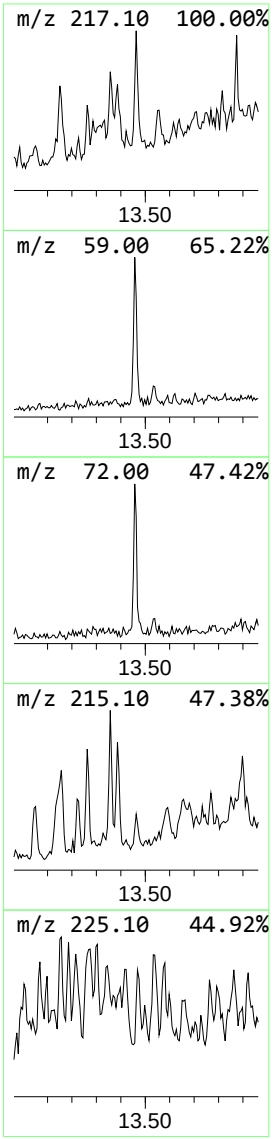
Peak Number 5 unknown13.463 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.463	6.60 ng	170407	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	25
2	1-Methyl-3-acetyl-4-hydroxyquino...	217	C12H11NO3	054289-76-8	25
3	Cobaltocene, 1,1'-dimethyl-	217	C12H14Co	012146-91-7	22
4	4-(4-tert-Butylphenyl)-1,3-thiaz...	232	C13H16N2S	081529-61-5	18
5	5,6,7,8-Tetrahydrothieno[2,3-b]q...	232	C13H16N2S	1000496-40-8	18





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BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

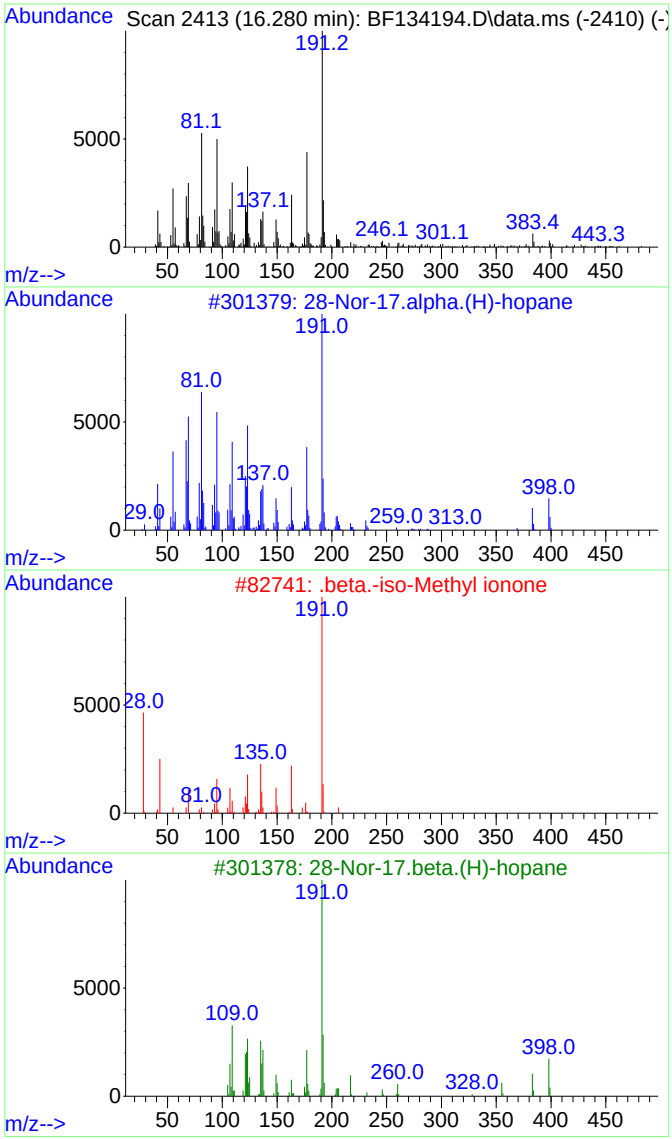
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

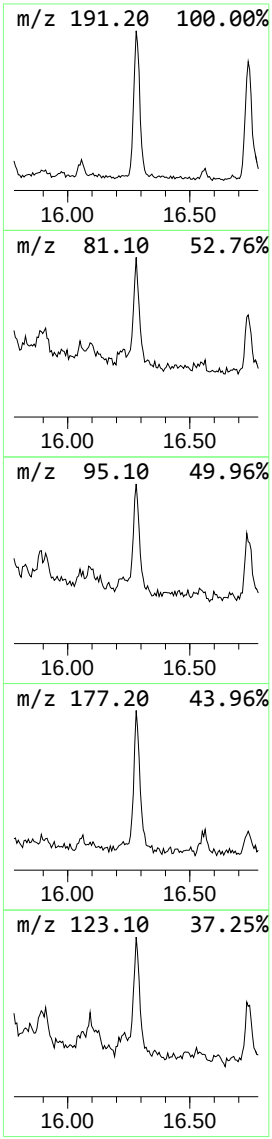
****

Peak Number 6 28-Nor-17.alpha.(H)-hopane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.280	20.00 ng	832752	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	95
2	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	58
3	28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	53
4	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	38
5	4,5-Dihydrothiazol-4-one, 2-(2-m...	222	C10H10N2O2S	022476-61-5	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071023\
Data File : BF134194.D
Acq On : 10 Jul 2023 19:31
Operator : CG\JU
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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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	10.592	2.3	ng	88172	3	9.881	777509	20.0
n-Hexadecanoic ...	11.904	3.3	ng	117785	4	11.374	724977	20.0
unknown12.698	12.698	2.1	ng	75204	4	11.374	724977	20.0
unknown13.151	13.151	6.1	ng	158146	5	14.039	516240	20.0
unknown13.463	13.463	6.6	ng	170407	5	14.039	516240	20.0
28-Nor-17.alpha...	16.280	20.0	ng	832752	6	15.557	832752	20.0