LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
Data File : BF134400.D
Acq On : 21 Jul 2023 14:31
Operator : CG\JU
Sample : 03638-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1

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: BF134400.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	12	rVB	329559	350317	26.75%	3.156%
2	5.081	506	509	517	rBV	15349	20905	1.60%	0.188%
3	5.475	572	576	596	rBV	1036820	1034781	79.00%	9.323%
4	6.110	681	684	688	rVB	18182	16304	1.24%	0.147%
5	6.475	742	746	753	rBV	1178127	1041308	79.50%	9.382%
6	6.534	753	756	763	rVB	32643	35327	2.70%	0.318%
7	6.834	804	807	816	rBV	411846	357700	27.31%	3.223%
8	7.398	899	903	906	rBV	819636	667717	50.98%	6.016%
9	8.116	1021	1025	1028	rBV	546611	457722	34.95%	4.124%
10	9.192	1204	1208	1211	rBV	1648347	1309801	100.00%	11.801%
11	9.875	1320	1324	1327	rBV	589838	529755	40.45%	4.773%
12	10.669	1455	1459	1469	rBV	976580	876716	66.94%	7.899%
13	11.369	1574	1578	1580	rBV	629791	535274	40.87%	4.823%
14	11.392	1580	1582	1587	rVB	94208	76579	5.85%	0.690%
15	11.898	1665	1668	1672	rBV2	197542	191466	14.62%	1.725%
16	11.980	1679	1682	1685	rBV	21482	22959	1.75%	0.207%
17	12.463	1760	1764	1770	rBV3	22889	32176	2.46%	0.290%
18	12.516	1770	1773	1779	rVB4	13872	17253	1.32%	0.155%
19	12.586	1782	1785	1789	rBV	182334	171992	13.13%	1.550%
20	12.686	1799	1802	1806	rBV2	54751	56869	4.34%	0.512%
21	12.822	1819	1825	1829	rVB	145405	159420	12.17%	1.436%
22	12.963	1845	1849	1852	rBV	1523319	1263371	96.46%	11.382%
23	13.045	1858	1863	1867	rVB5	14866	23989	1.83%	0.216%
24	13.127	1874	1877	1879	rBV4	14047	17230	1.32%	0.155%
25	13.151	1879	1881	1885	rVB2	22315	26473	2.02%	0.239%
26	13.257	1895	1899	1906	rVB2	26322	37432	2.86%	0.337%
27	13.533	1942	1946	1949	rBV2	20052	29946	2.29%	0.270%
28	13.669	1965	1969	1972	rVB	21586	22697	1.73%	0.204%
29	13.868	2000	2003	2008	rVB3	27309	35228	2.69%	0.317%
30	13.927	2008	2013	2024	rBV4	40091	120225	9.18%	1.083%
31	14.027	2024	2030	2033	rVV2	457655	505432	38.59%	4.554%
32	14.057	2033	2035	2041	rVB	76642	70037	5.35%	0.631%
33	14.186	2054	2057	2062	rBV2	33226	36998	2.82%	0.333%
34	14.421	2093	2097	2099	rVB	18936	16090	1.23%	0.145%
35	14.492	2106	2109	2112	rVB3	23968	20917	1.60%	0.188%
36	14.810	2160	2163	2167	rVB	14554	16283	1.24%	0.147%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
Data File : BF134400.D
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Operator : CG\JU
Sample : 03638-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1

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	14.957	2185	2188	2195	rVB4	35861	39595	3.02%	0.357%
38	15.092	2207	2211	2214	rBV	52527	80005	6.11%	0.721%
39	15.157	2219	2222	2226	rVB3	21085	24608	1.88%	0.222%
40	15.310	2242	2248	2252	rBV8	13459	28472	2.17%	0.257%
41	15.404	2261	2264	2270	rVB	29821	40881	3.12%	0.368%
42	15.468	2271	2275	2281	rVB	39644	54757	4.18%	0.493%
43	15.533	2281	2286	2295	rBV	253614	363871	27.78%	3.278%
44	15.762	2322	2325	2332	rVB8	12376	20854	1.59%	0.188%
45	16.010	2363	2367	2371	rVB5	16989	23616	1.80%	0.213%
46	16.851	2506	2510	2514	rBV7	9293	18046	1.38%	0.163%
47	17.086	2541	2550	2558	rVB3	20873	52703	4.02%	0.475%
48	17.174	2558	2565	2572	rBV9	16708	46659	3.56%	0.420%
49	17.268	2575	2581	2589	rVB8	26431	59442	4.54%	0.536%
50	17.556	2624	2630	2640	rVB3	16466	41235	3.15%	0.372%

Sum of corrected areas: 11099433

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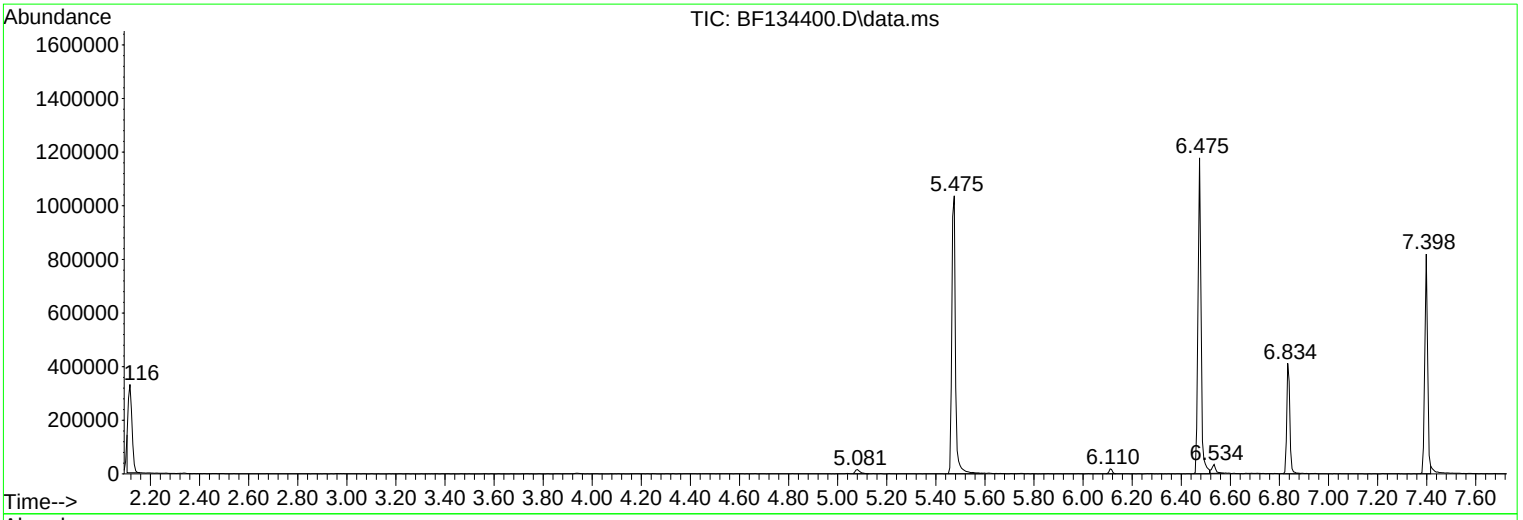
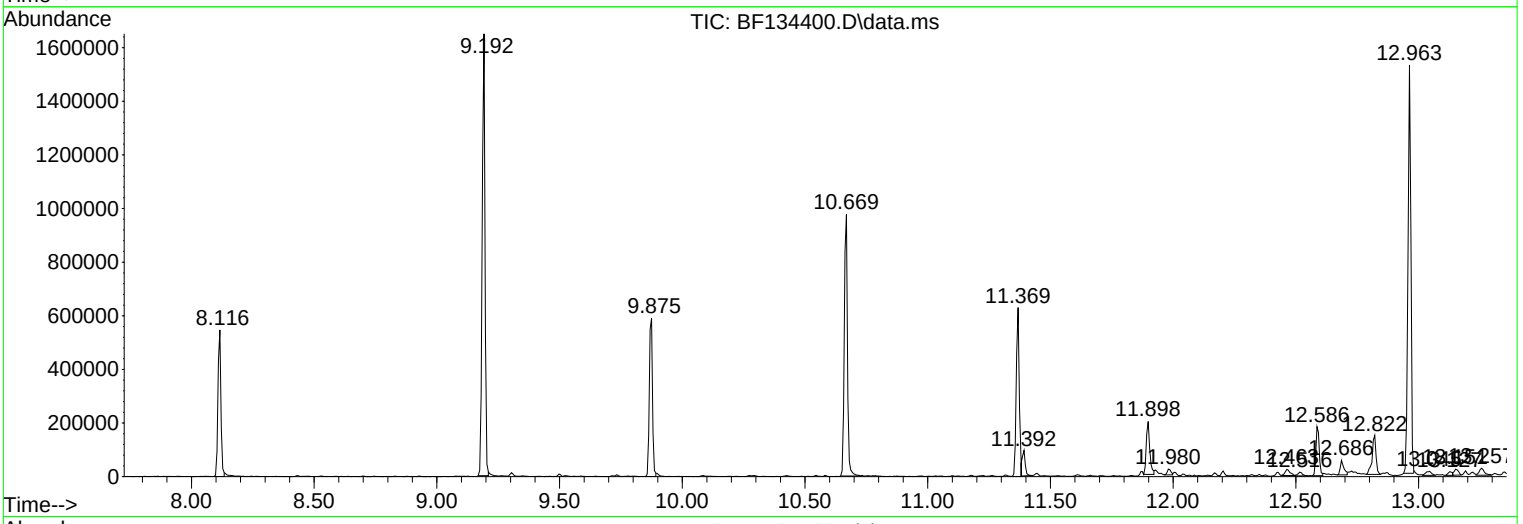
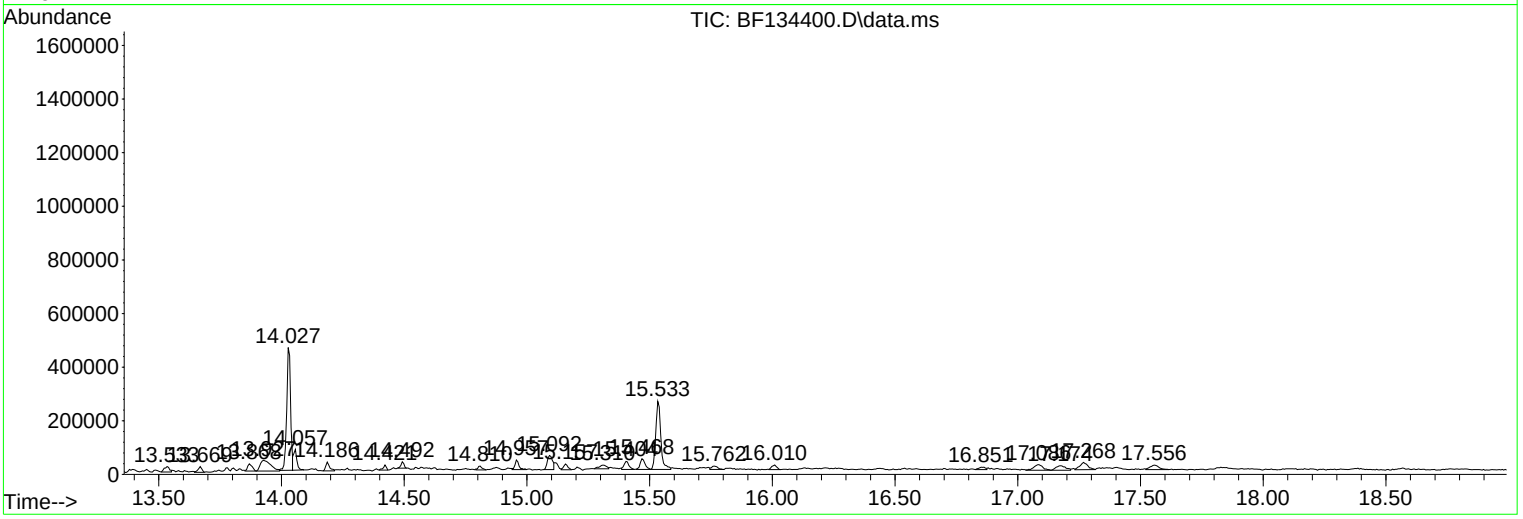
Instrument :
BNA_F
ClientSampleId :
TP1

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\BF072123\
Data File : BF134400.D
Acq On : 21 Jul 2023 14:31
Operator : CG\JU
Sample : 03638-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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

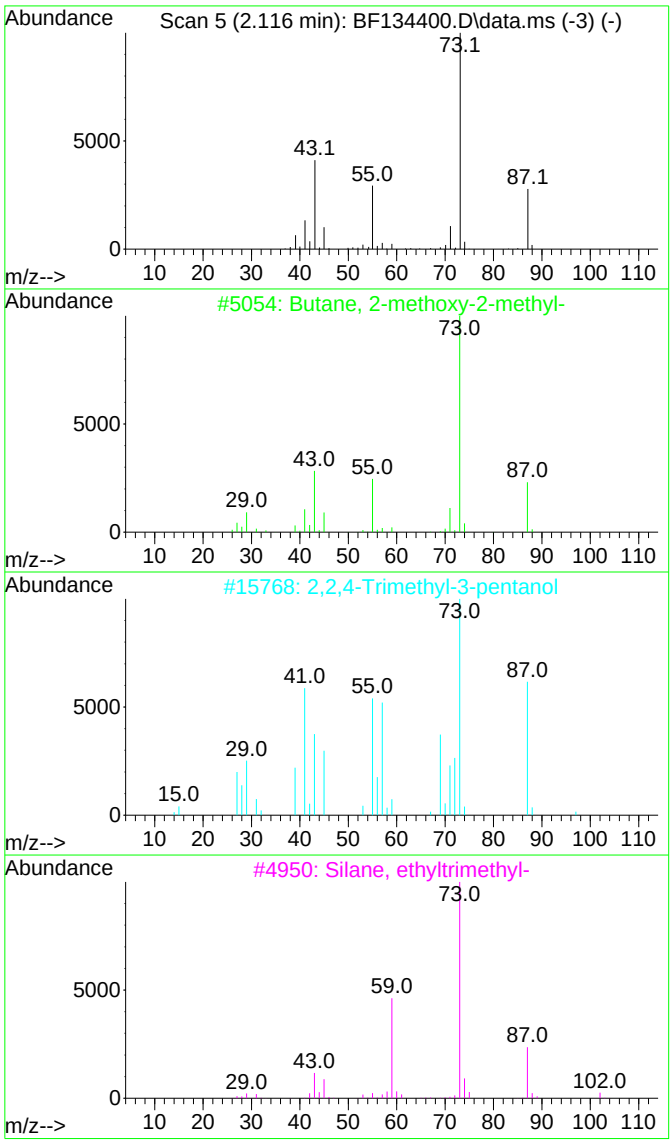
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

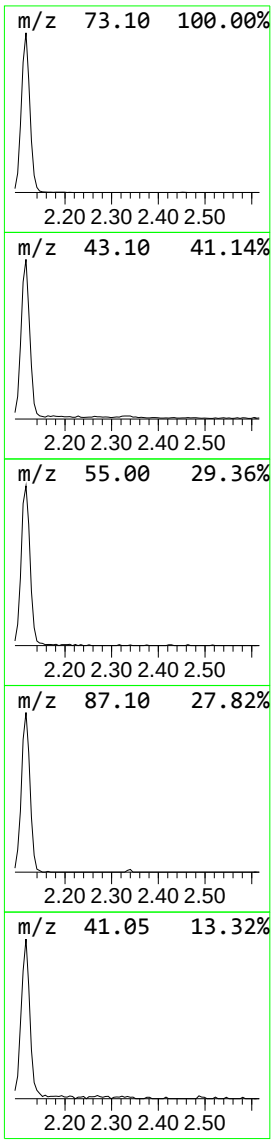
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	19.59 ng	350317	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	33
4	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
Data File : BF134400.D
Acq On : 21 Jul 2023 14:31
Operator : CG\JU
Sample : 03638-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1

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

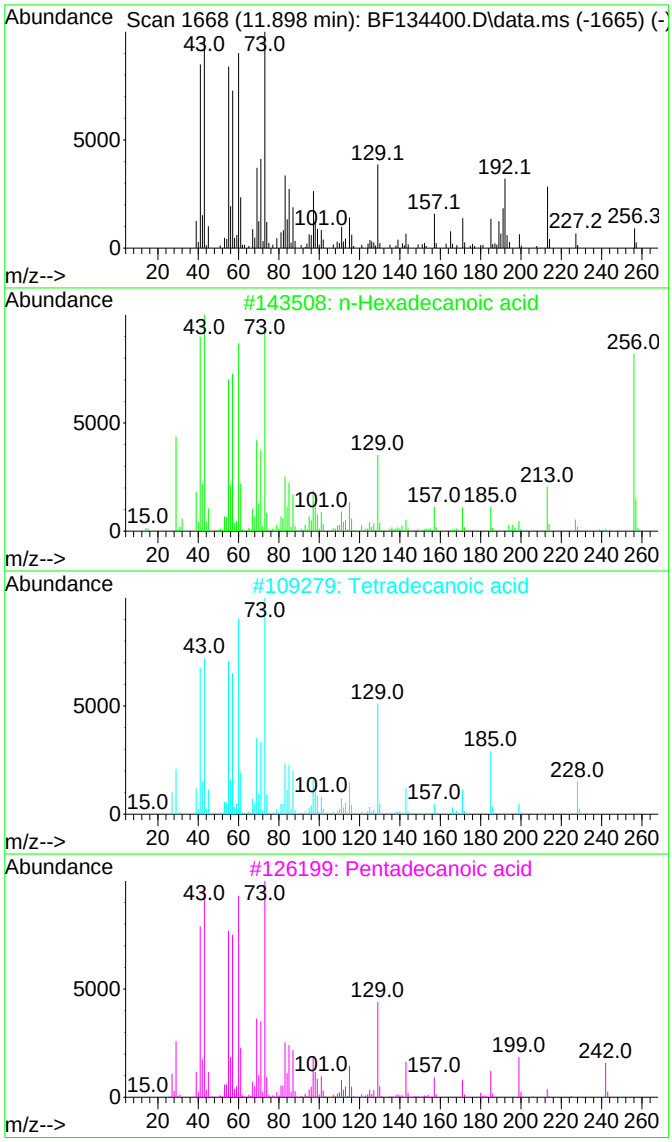
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

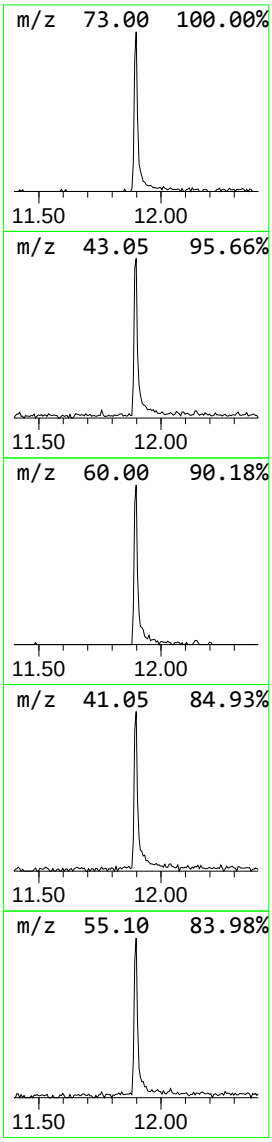
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	7.15 ng	191466	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	74
5	Undecanoic acid	186	C11H22O2	000112-37-8	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
Data File : BF134400.D
Acq On : 21 Jul 2023 14:31
Operator : CG\JU
Sample : 03638-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1

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

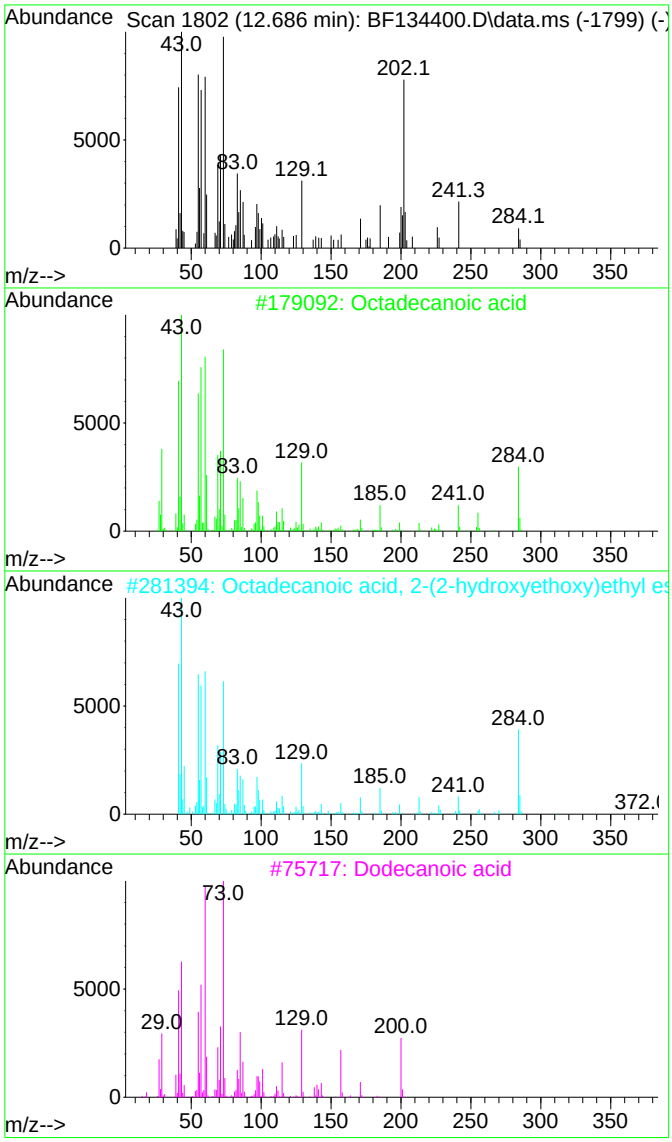
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

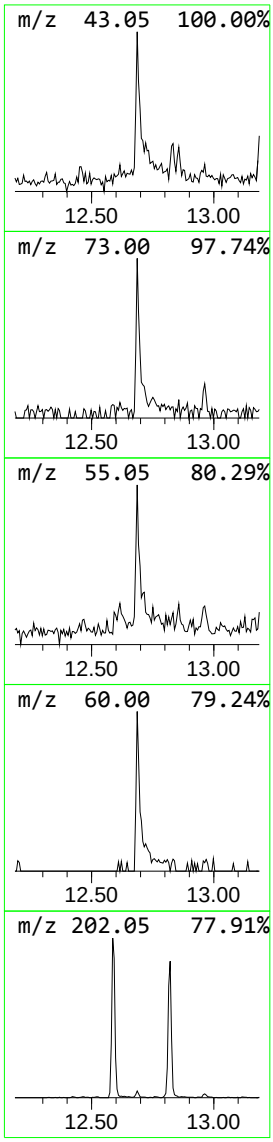
****

Peak Number 3 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.686	2.12 ng	56869	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	53
3	Dodecanoic acid	200	C12H24O2	000143-07-7	50
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	45
5	Tridecanoic acid	214	C13H26O2	000638-53-9	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
Data File : BF134400.D
Acq On : 21 Jul 2023 14:31
Operator : CG\JU
Sample : 03638-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1

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

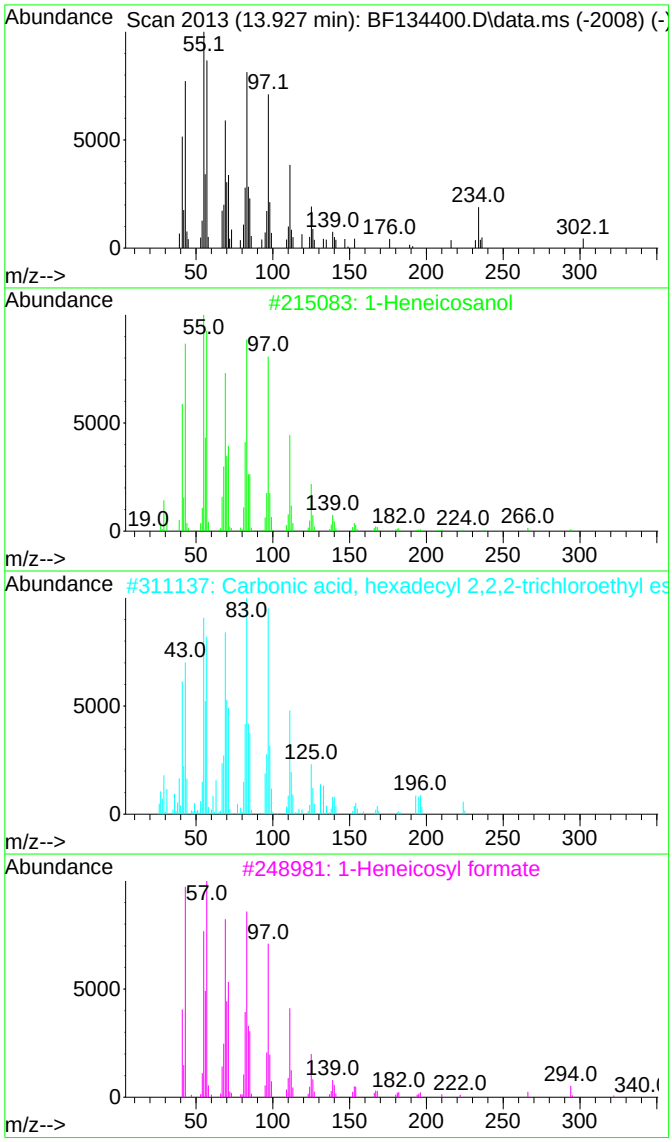
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

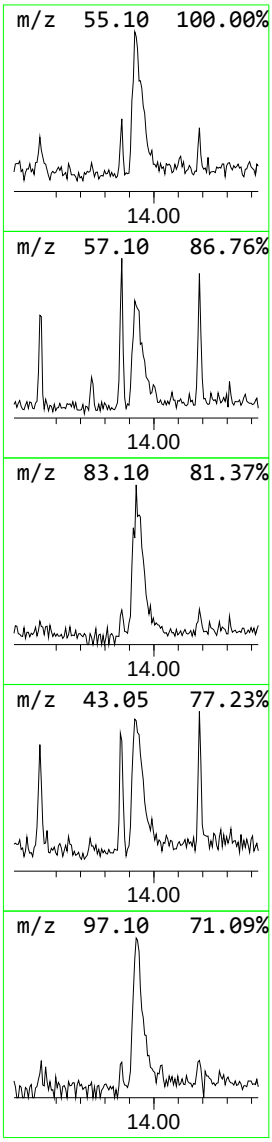
****

Peak Number 4 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	4.76 ng	120225	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	90
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	87
4	1-Docosene	308	C22H44	001599-67-3	87
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	87





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Data File : BF134400.D
Acq On : 21 Jul 2023 14:31
Operator : CG\JU
Sample : 03638-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1

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

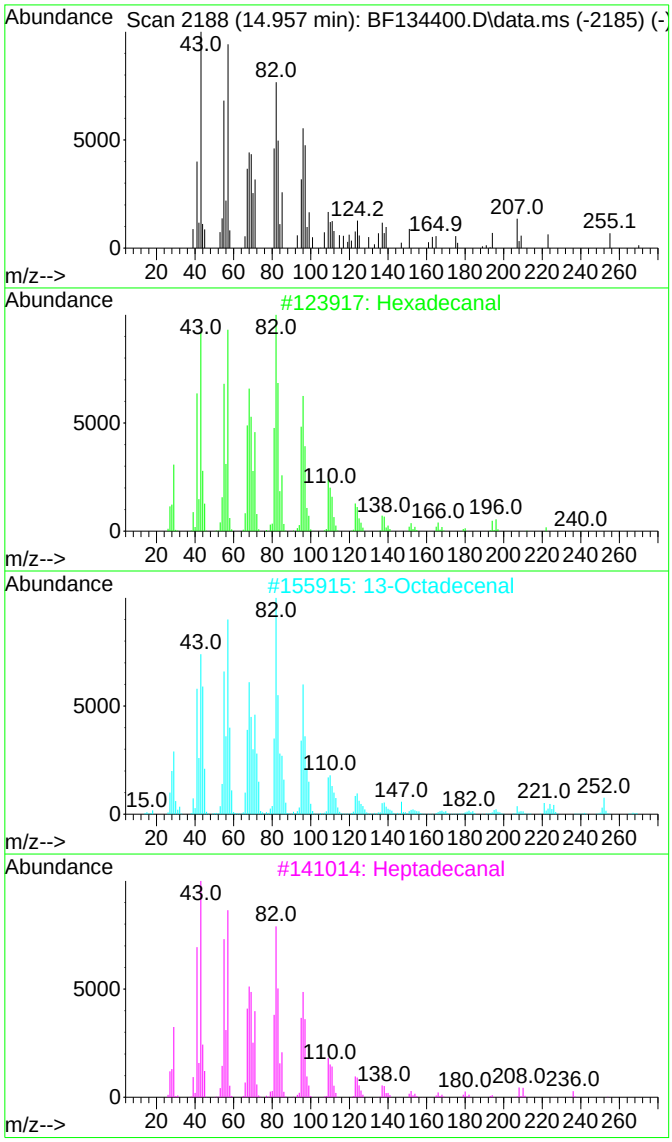
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

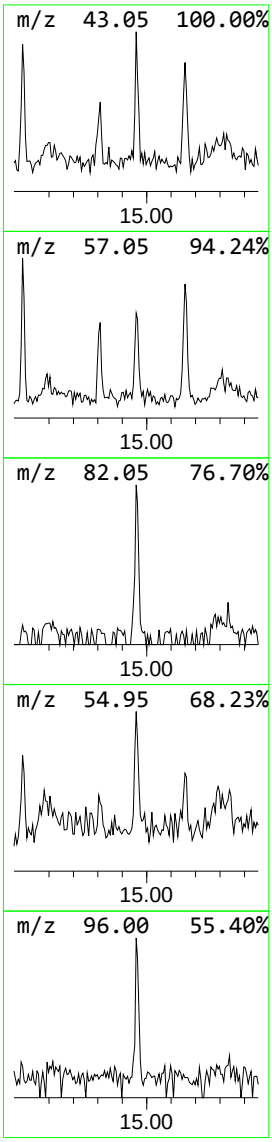
****

Peak Number 5 Hexadecanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.957	2.18 ng	39595	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanal	240	C16H32O	000629-80-1	81
2	13-Octadecenal	266	C18H34O	056554-90-6	80
3	Heptadecanal	254	C17H34O	1000376-70-0	76
4	Octadecanal	268	C18H36O	000638-66-4	76
5	17-Octadecenal	266	C18H34O	056554-86-0	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
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Sample : 03638-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1

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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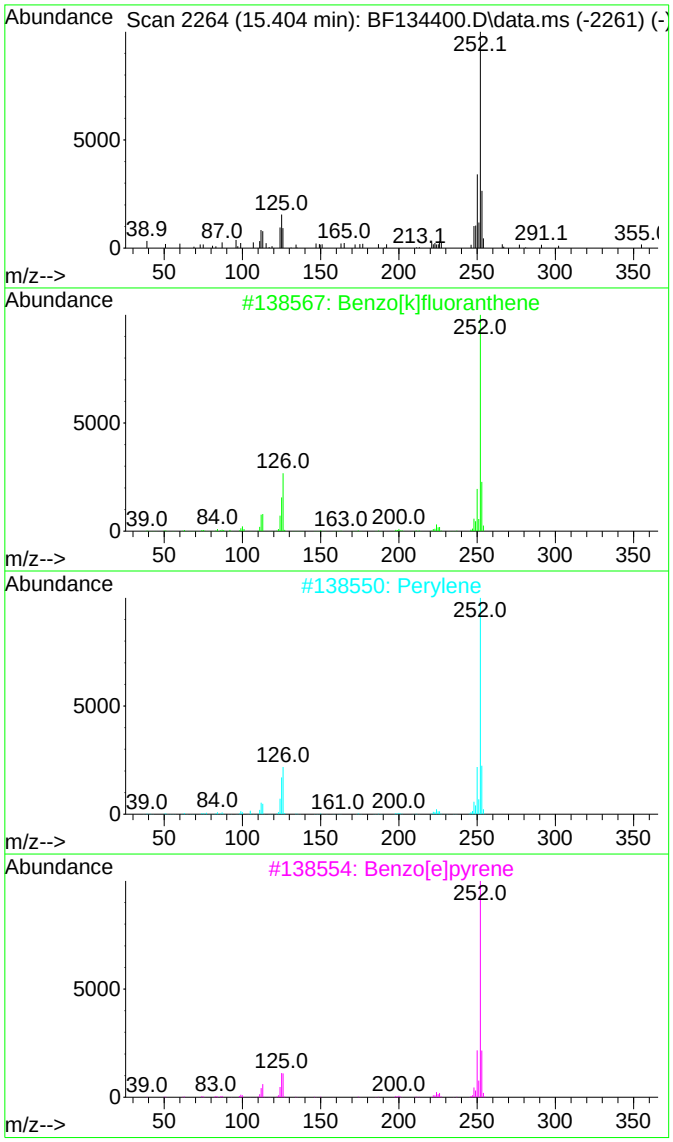
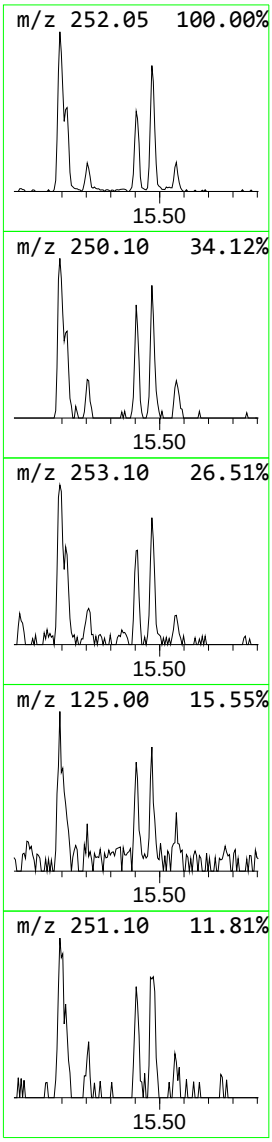
Peak Number 6 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.404	2.25 ng	40881	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	89
2	Perylene	252	C20H12	000198-55-0	89
3	Benzo[e]pyrene	252	C20H12	000192-97-2	76
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	76
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
Data File : BF134400.D
Acq On : 21 Jul 2023 14:31
Operator : CG\JU
Sample : 03638-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1

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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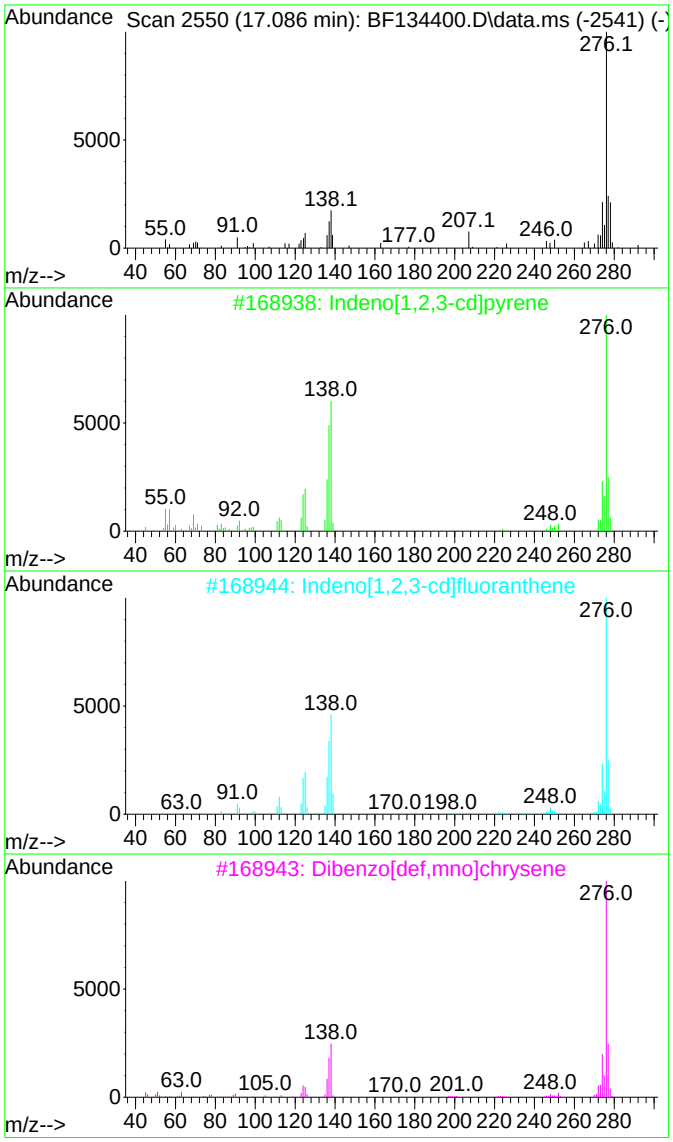
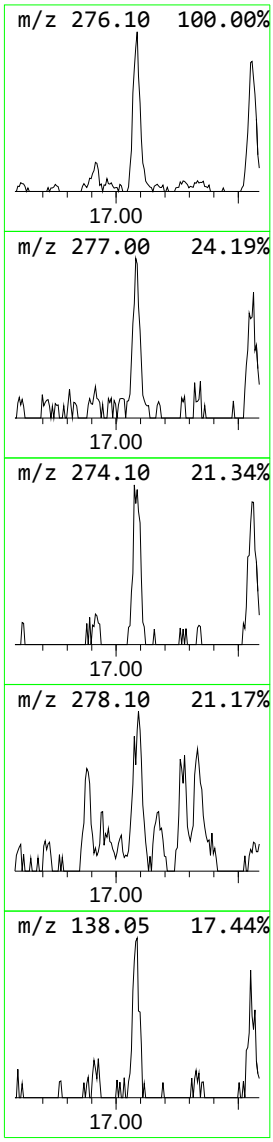
Peak Number 7 Indeno[1,2,3-cd]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.086	2.90 ng	52703	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	81
2	Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	76
3	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	76
4	Benzo[ghi]perylene	276	C22H12	000191-24-2	76
5	Naphthalen-1-yl-(3-nitro-benzyli...	276	C17H12N2O2	200421-53-0	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
Data File : BF134400.D
Acq On : 21 Jul 2023 14:31
Operator : CG\JU
Sample : 03638-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1

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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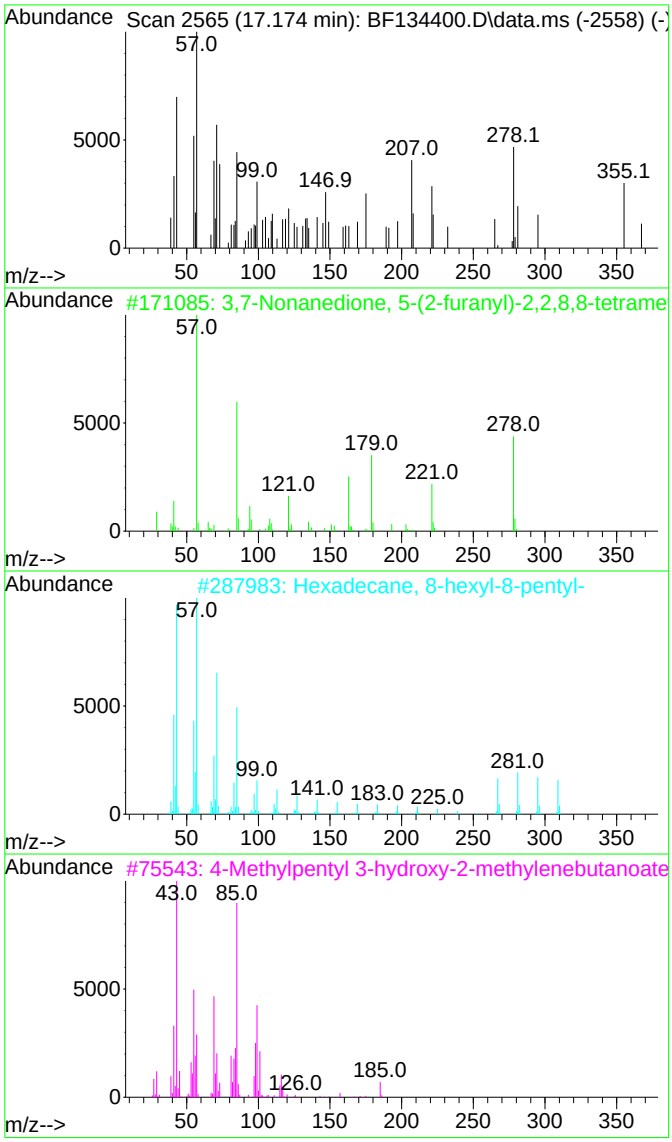
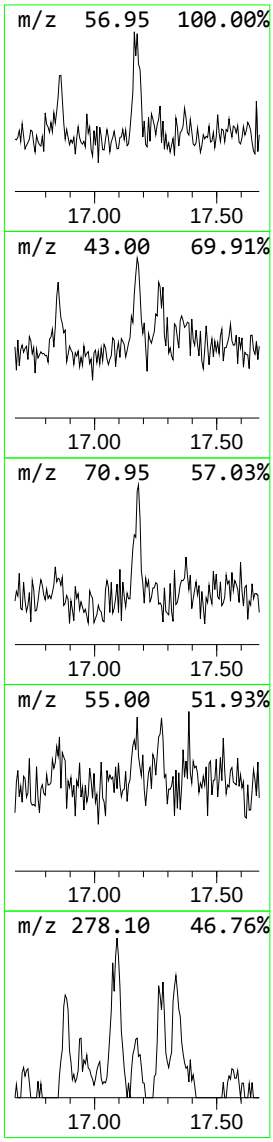
Peak Number 8 unknown17.174 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.174	2.56 ng	46659	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,7-Nonanedione, 5-(2-furanyl)-2...	278	C17H26O3	1010319-41-4	27
2	Hexadecane, 8-hexyl-8-pentyl-	380	C27H56	055282-29-6	14
3	4-Methylpentyl 3-hydroxy-2-methy...	200	C11H20O3	1000413-53-1	10
4	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	10
5	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	10





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Acq On : 21 Jul 2023 14:31
Operator : CG\JU
Sample : 03638-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1

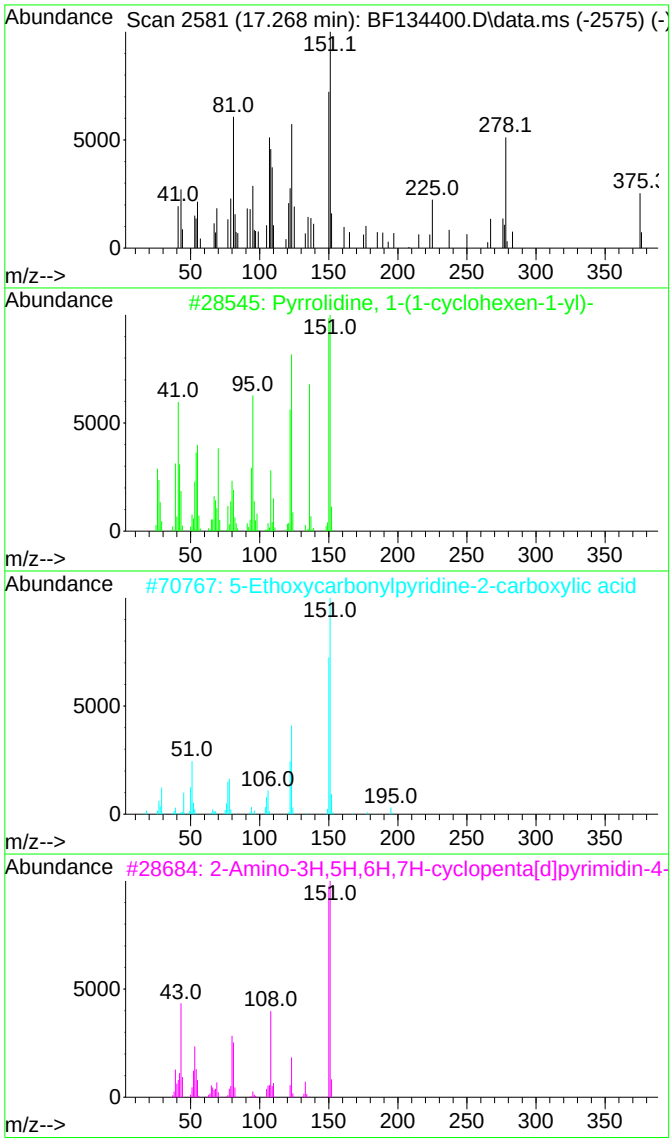
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

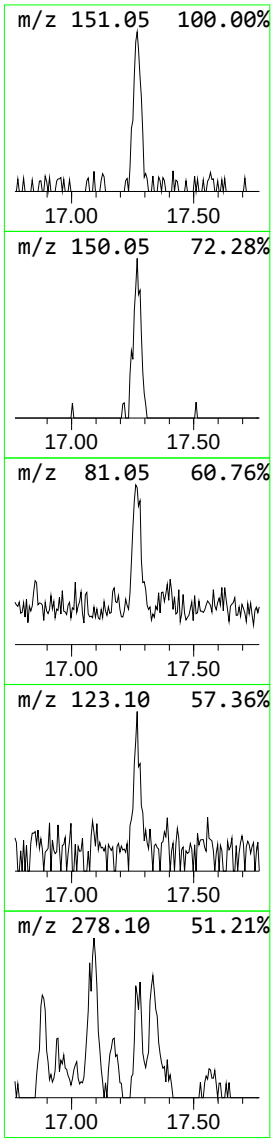
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Pyrrolidine, 1-(1-cyclohexe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.268	3.27 ng	59442	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrrolidine, 1-(1-cyclohexen-1-yl)-	151	C10H17N	001125-99-1	50
2	5-Ethoxycarbonylpyridine-2-carbo...	195	C9H9NO4	017880-34-1	38
3	2-Amino-3H,5H,6H,7H-cyclopenta[d...	151	C7H9N3O	033081-06-0	38
4	2-(2-Acetoxyethyl)-3,4-dihydro-6...	278	C16H22O4	1010432-27-8	38
5	Phenoxyacetamide	151	C8H9NO2	000621-88-5	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
Data File : BF134400.D
Acq On : 21 Jul 2023 14:31
Operator : CG\JU
Sample : 03638-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1

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

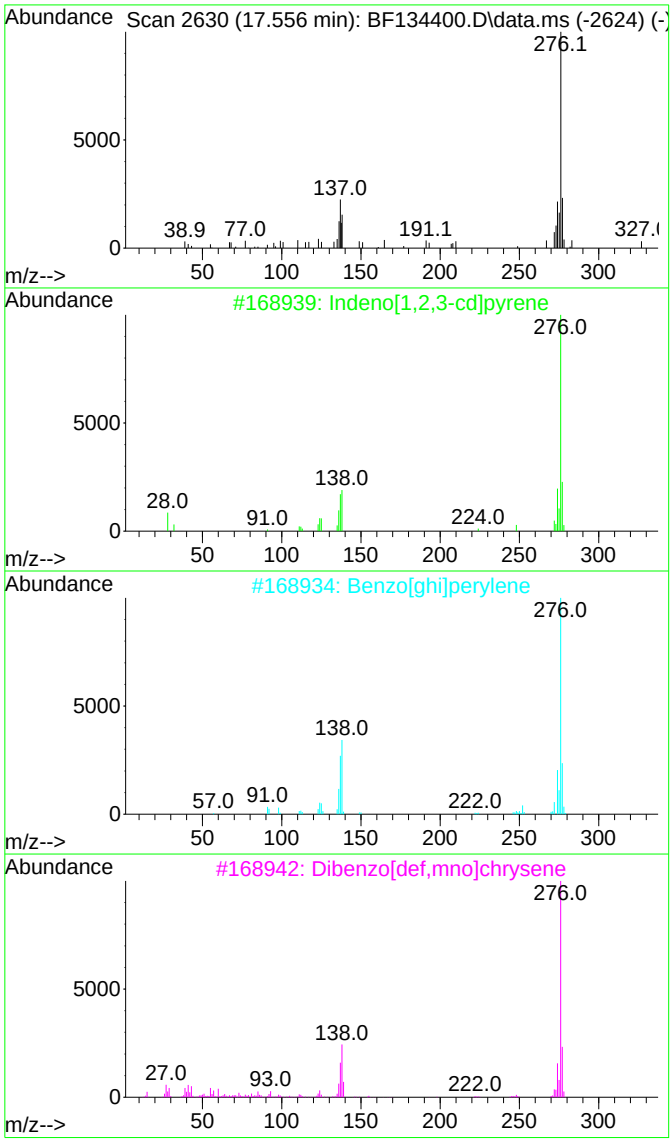
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

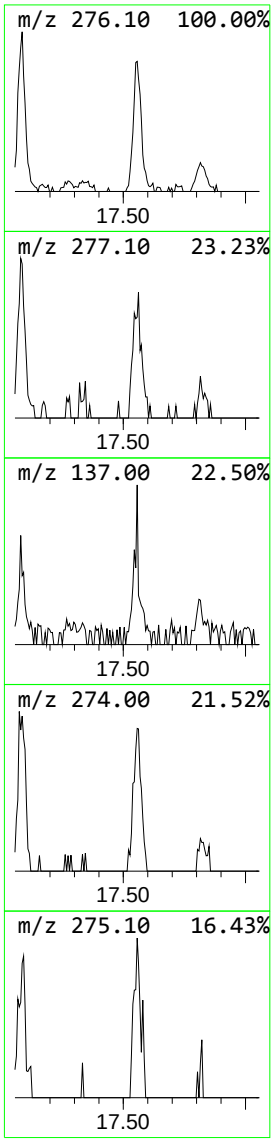
****

Peak Number 10 Indeno[1,2,3-cd]fluoranthene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.557	2.27 ng	41235	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	81
2	Benzo[ghi]perylene	276	C22H12	000191-24-2	64
3	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	59
4	Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	53
5	1H-Cyclopenta[4,5]pyrido[1,2-a]b...	276	C17H16N4	329707-31-5	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
Data File : BF134400.D
Acq On : 21 Jul 2023 14:31
Operator : CG\JU
Sample : 03638-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1

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
Butane, 2-metho...	2.116	19.6	ng	350317	1	6.834	357700	20.0
n-Hexadecanoic ...	11.898	7.2	ng	191466	4	11.369	535274	20.0
Octadecanoic acid	12.686	2.1	ng	56869	4	11.369	535274	20.0
1-Heneicosanol	13.927	4.8	ng	120225	5	14.027	505432	20.0
Hexadecanal	14.957	2.2	ng	39595	6	15.533	363871	20.0
Benzo[e]pyrene	15.404	2.3	ng	40881	6	15.533	363871	20.0
Indeno[1,2,3-cd...	17.086	2.9	ng	52703	6	15.533	363871	20.0
unknown17.174	17.174	2.6	ng	46659	6	15.533	363871	20.0
Pyrrolidine, 1-...	17.268	3.3	ng	59442	6	15.533	363871	20.0
Indeno[1,2,3-cd...	17.557	2.3	ng	41235	6	15.533	363871	20.0