LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071423\
Data File : BF134308.D
Acq On : 15 Jul 2023 01:30
Operator : CG\JU
Sample : 03597-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-44-(2-5)

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: BF134308.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.081	505	509	517	rVB	18876	27032	1.59%	0.195%
2	5.475	572	576	590	rBV	1630052	1576931	92.75%	11.358%
3	6.481	742	747	760	rBV	1632162	1584245	93.18%	11.411%
4	6.675	777	780	793	rBV	40149	61281	3.60%	0.441%
5	6.840	805	808	818	rBV	629078	491591	28.91%	3.541%
6	7.404	900	904	907	rBV	1223081	1003233	59.01%	7.226%
7	8.122	1022	1026	1029	rBV	725216	612842	36.04%	4.414%
8	9.198	1205	1209	1212	rBV	2156099	1700246	100.00%	12.246%
9	9.310	1225	1228	1235	rVB	498556	485076	28.53%	3.494%
10	9.881	1321	1325	1328	rBV	771727	652466	38.37%	4.700%
11	10.675	1456	1460	1475	rBV	1278910	1183468	69.61%	8.524%
12	11.375	1575	1579	1581	rBV	759465	626206	36.83%	4.510%
13	11.398	1581	1583	1588	rVV	85626	75726	4.45%	0.545%
14	11.445	1588	1591	1595	rVB2	20233	26924	1.58%	0.194%
15	11.904	1666	1669	1676	rBV2	198195	189848	11.17%	1.367%
16	12.475	1761	1766	1771	rVB2	95152	117033	6.88%	0.843%
17	12.592	1783	1786	1790	rBV	145256	146160	8.60%	1.053%
18	12.692	1801	1803	1808	rBV3	36319	43294	2.55%	0.312%
19	12.827	1820	1826	1831	rBV	144693	162547	9.56%	1.171%
20	12.969	1846	1850	1858	rVB	1602988	1390588	81.79%	10.016%
21	13.045	1859	1863	1868	rVB3	14405	24676	1.45%	0.178%
22	13.263	1896	1900	1903	rVB2	20491	22335	1.31%	0.161%
23	13.674	1967	1970	1974	rVB	19141	20558	1.21%	0.148%
24	13.780	1983	1988	1991	rBV5	15485	23382	1.38%	0.168%
25	13.904	2002	2009	2022	rVB6	45891	138559	8.15%	0.998%
26	14.033	2024	2031	2034	rBV2	558515	611858	35.99%	4.407%
27	14.063	2034	2036	2044	rVB	89928	90726	5.34%	0.653%
28	14.192	2055	2058	2061	rBV3	21174	25597	1.51%	0.184%
29	14.427	2095	2098	2101	rVB2	21292	21465	1.26%	0.155%
30	14.498	2107	2110	2117	rBV8	18139	30918	1.82%	0.223%
31	15.098	2207	2212	2215	rBV	68176	106283	6.25%	0.766%
32	15.410	2261	2265	2272	rVB	45568	58040	3.41%	0.418%
33	15.474	2272	2276	2281	rBV	52871	72696	4.28%	0.524%
34	15.539	2282	2287	2300	rVV	294575	407108	23.94%	2.932%
35	17.080	2547	2549	2556	rVB2	16425	29168	1.72%	0.210%
36	17.557	2623	2630	2637	rVB3	15933	43589	2.56%	0.314%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071423\
Data File : BF134308.D
Acq On : 15 Jul 2023 01:30
Operator : CG\JU
Sample : 03597-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-44-(2-5)

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

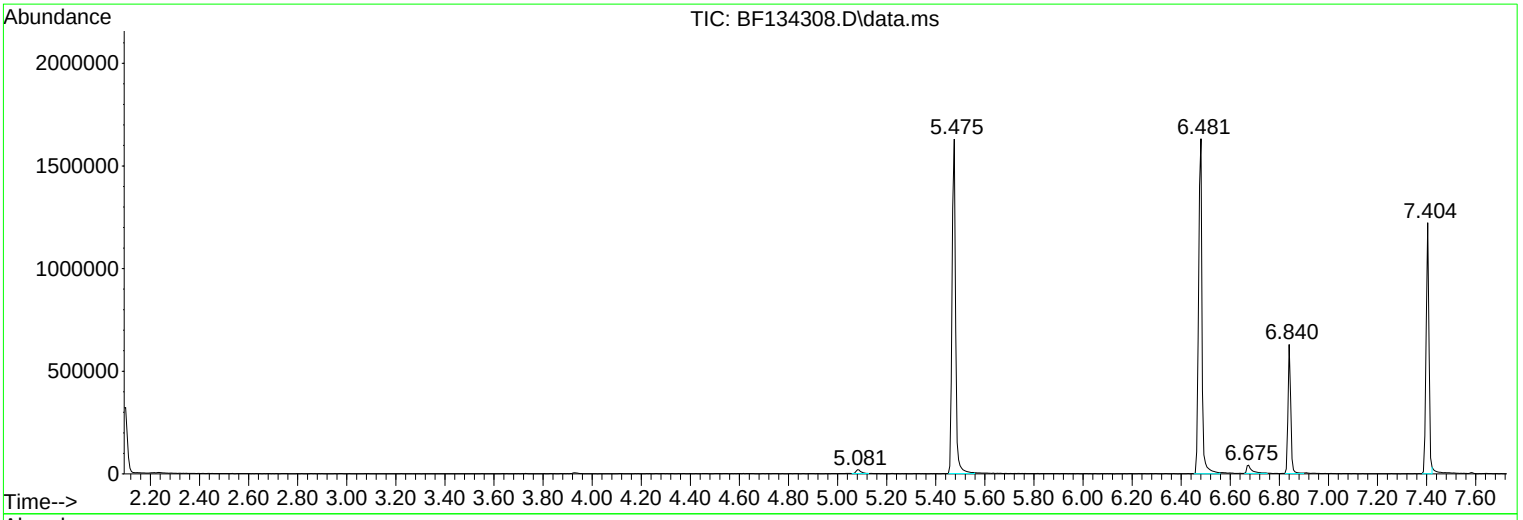
Sum of corrected areas: 13883695

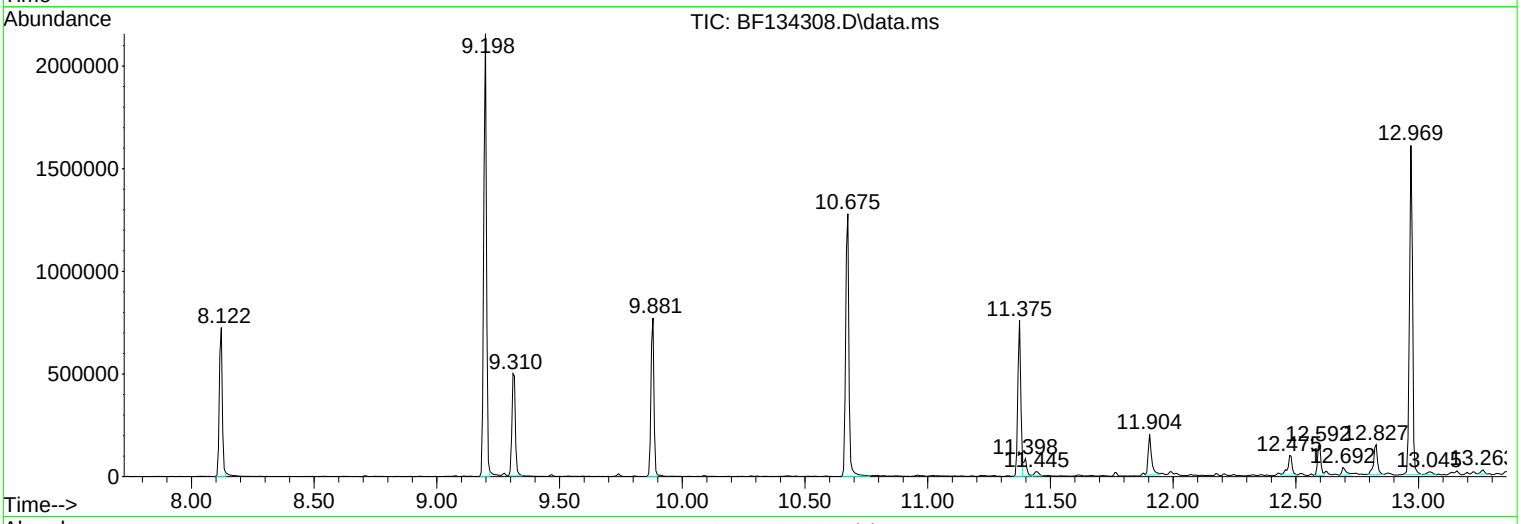
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071423\
Data File : BF134308.D
Acq On : 15 Jul 2023 01:30
Operator : CG\JU
Sample : 03597-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

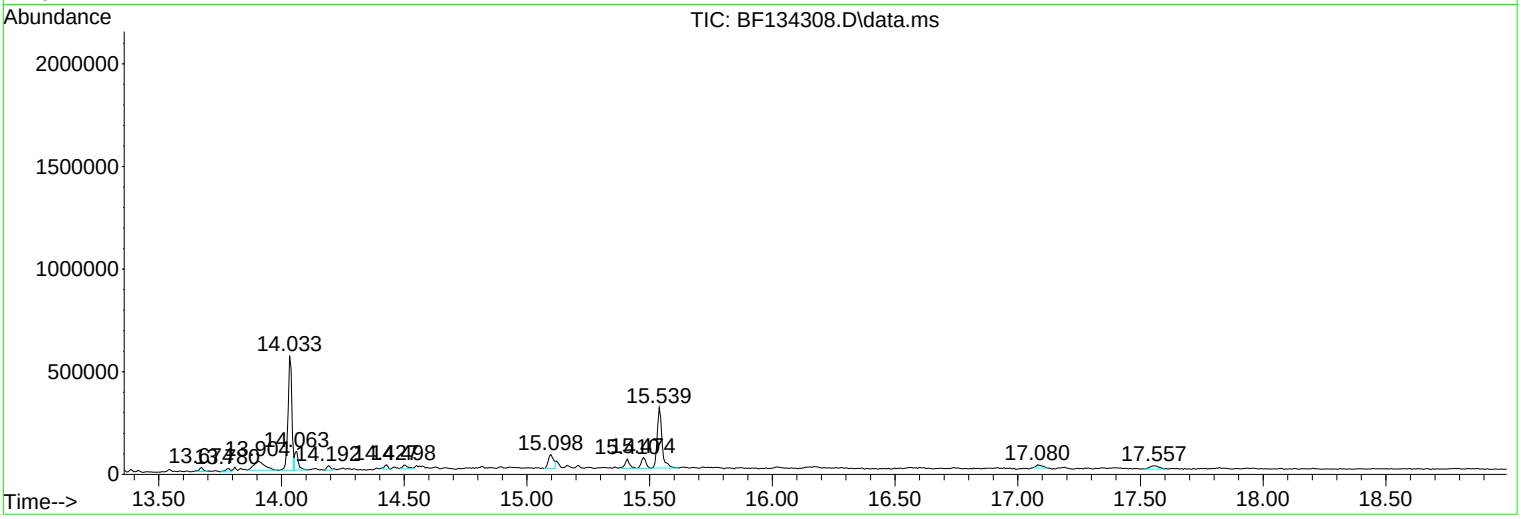
Instrument :
BNA_F
ClientSampleId :
RB-44-(2-5)

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\BF071423\
Data File : BF134308.D
Acq On : 15 Jul 2023 01:30
Operator : CG\JU
Sample : 03597-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-44-(2-5)

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

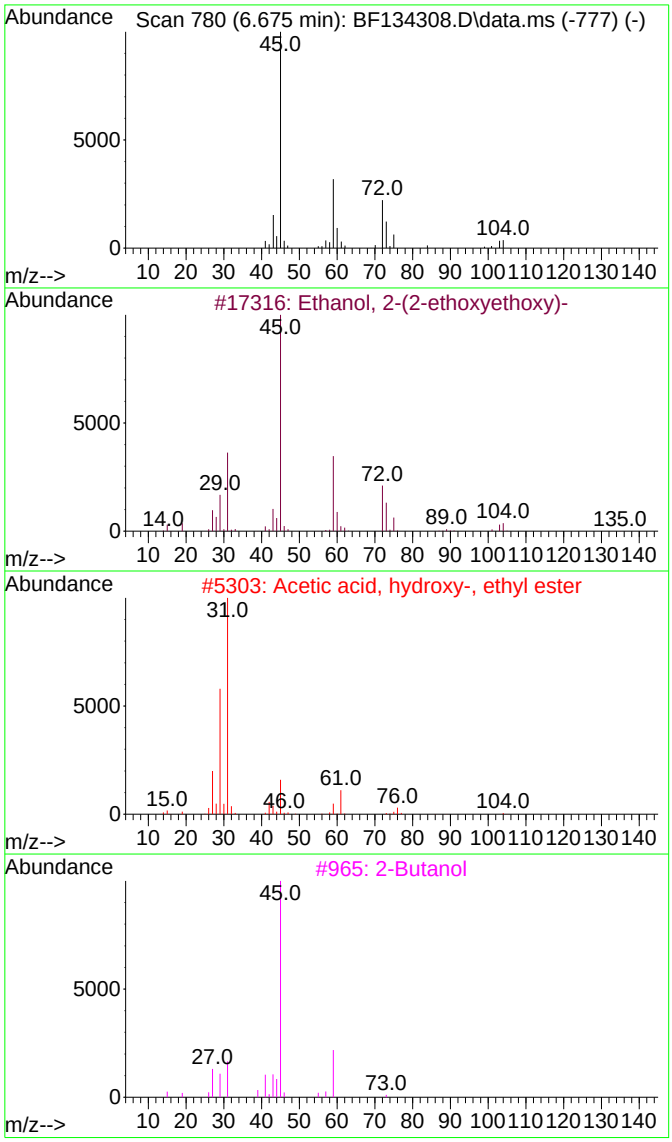
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

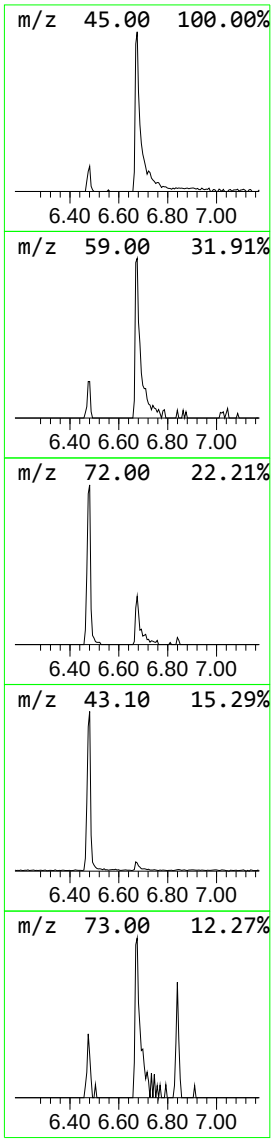
****

Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.675	2.49 ng	61281	1,4-Dichlorobenzene-d4	6.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	Acetic acid, hydroxy-, ethyl ester	104	C4H8O3	000623-50-7	42
3	2-Butanol	74	C4H10O	000078-92-2	40
4	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	39
5	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071423\
Data File : BF134308.D
Acq On : 15 Jul 2023 01:30
Operator : CG\JU
Sample : 03597-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-44-(2-5)

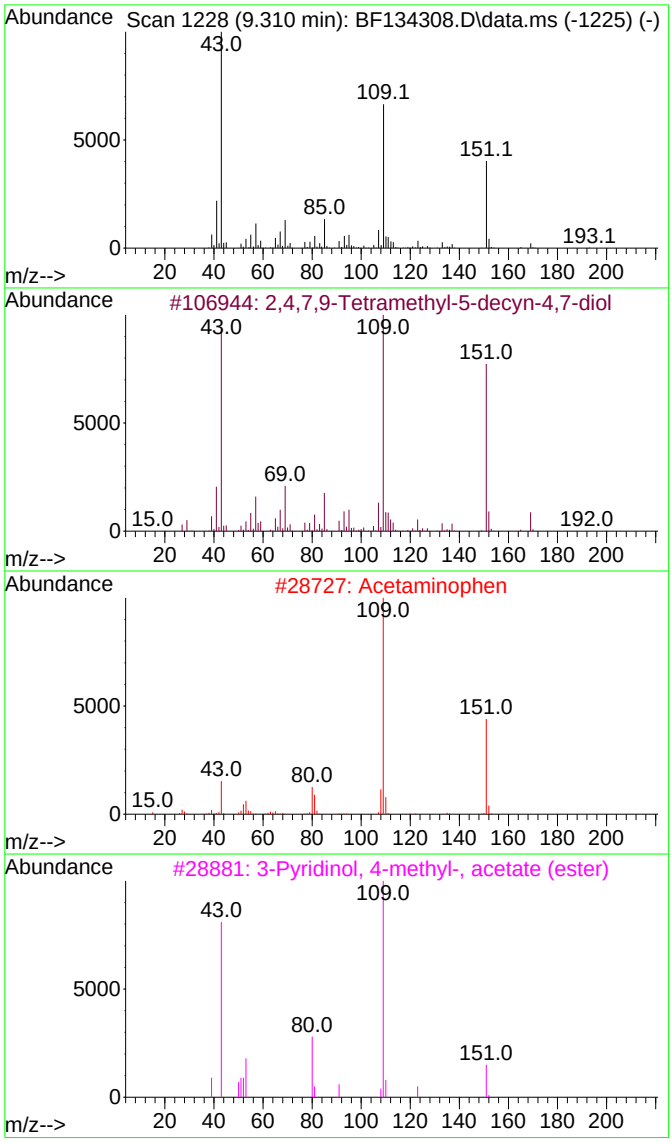
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

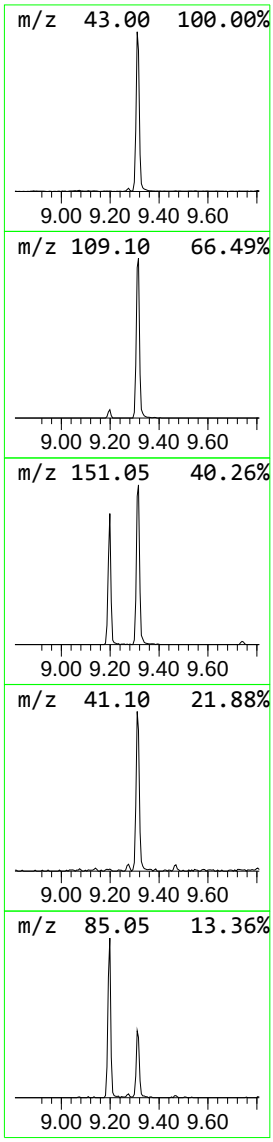
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.310	14.87 ng	485076	Acenaphthene-d10	9.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	86
2	Acetaminophen	151	C8H9NO2	000103-90-2	58
3	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	53
4	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	42
5	1-(1,2,3-Trimethyl-cyclopent-2-e...	152	C10H16O	070987-81-4	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071423\
Data File : BF134308.D
Acq On : 15 Jul 2023 01:30
Operator : CG\JU
Sample : 03597-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-44-(2-5)

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

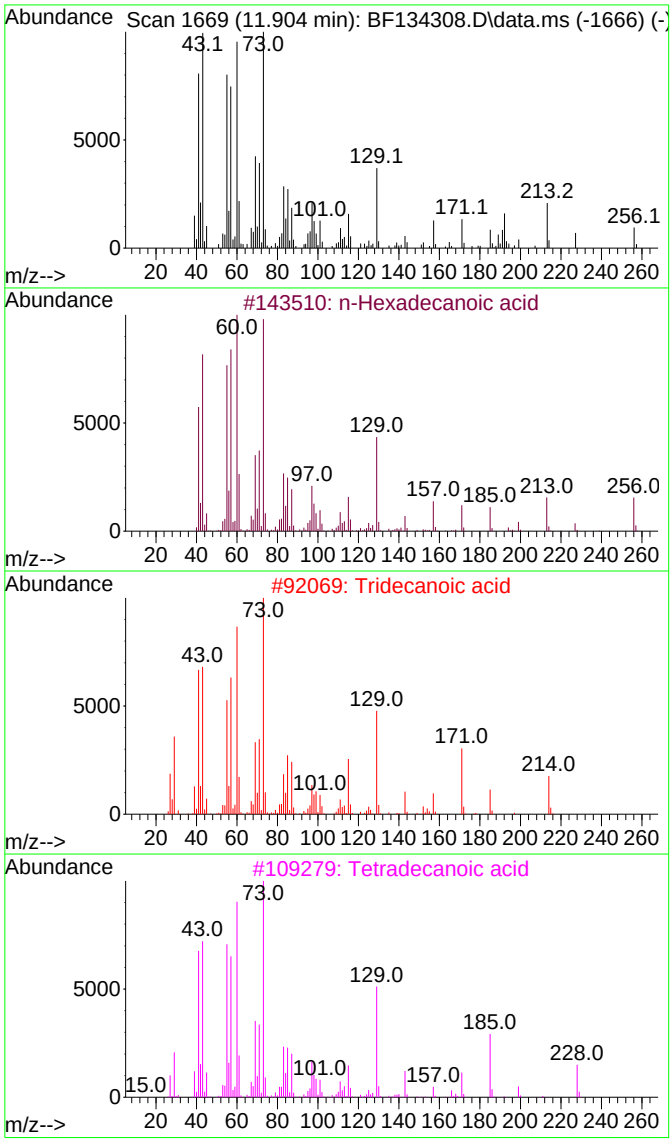
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

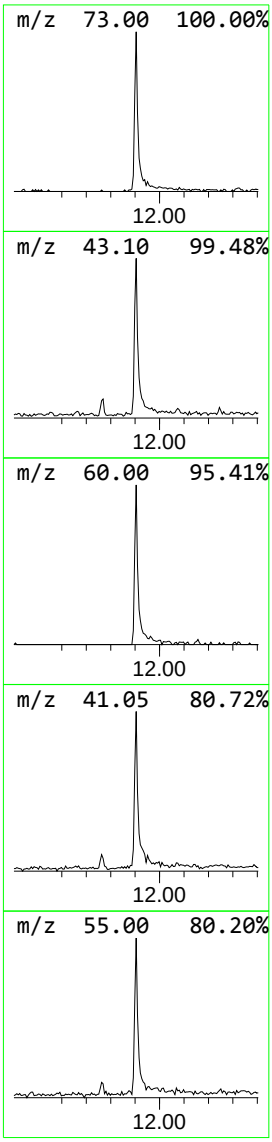
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	6.06 ng	189848	Phenanthrene-d10	11.375

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	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071423\
Data File : BF134308.D
Acq On : 15 Jul 2023 01:30
Operator : CG\JU
Sample : 03597-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-44-(2-5)

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

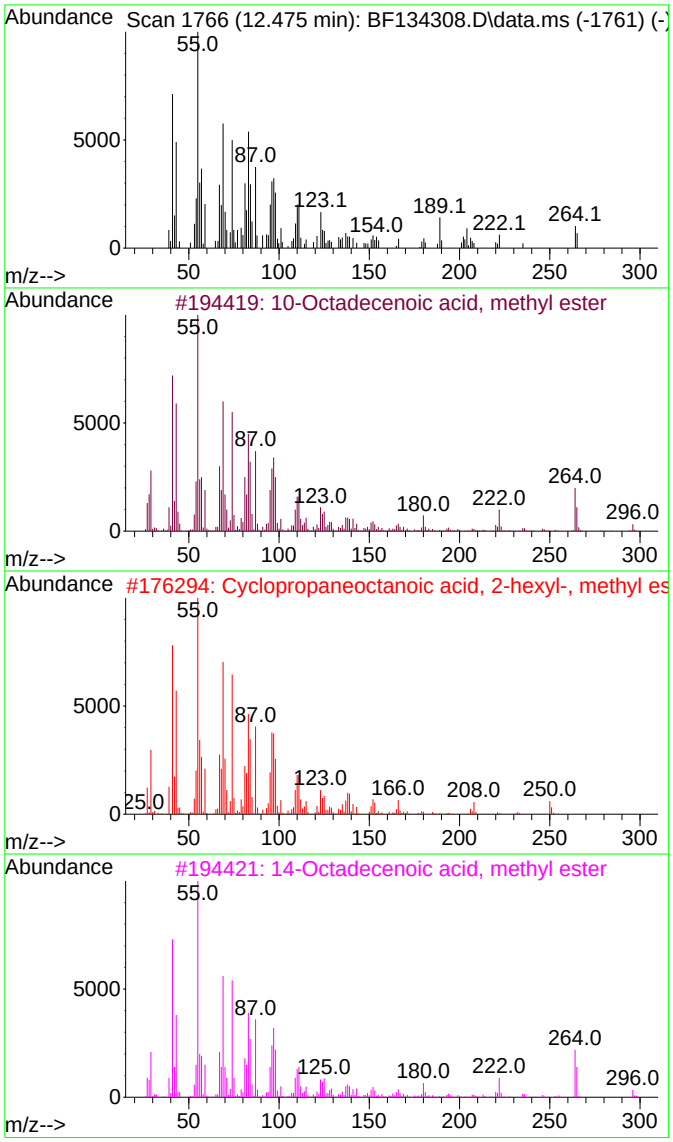
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

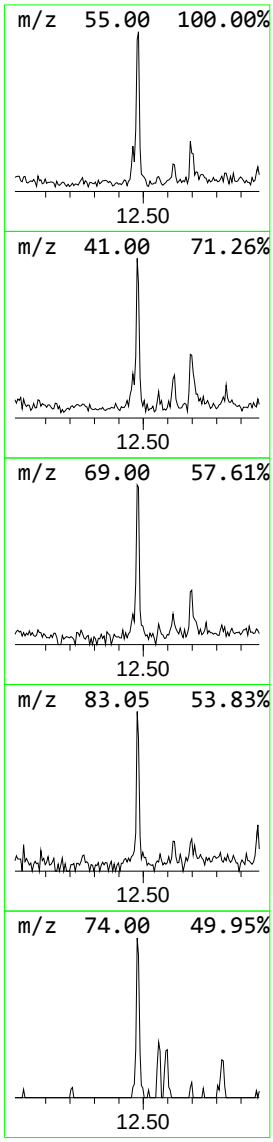
****

Peak Number 4 10-Octadecenoic acid, methy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.475	3.74 ng	117033	Phenanthrene-d10	11.375

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
2	Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	90
3	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	90
4	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	87
5	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071423\
Data File : BF134308.D
Acq On : 15 Jul 2023 01:30
Operator : CG\JU
Sample : 03597-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-44-(2-5)

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

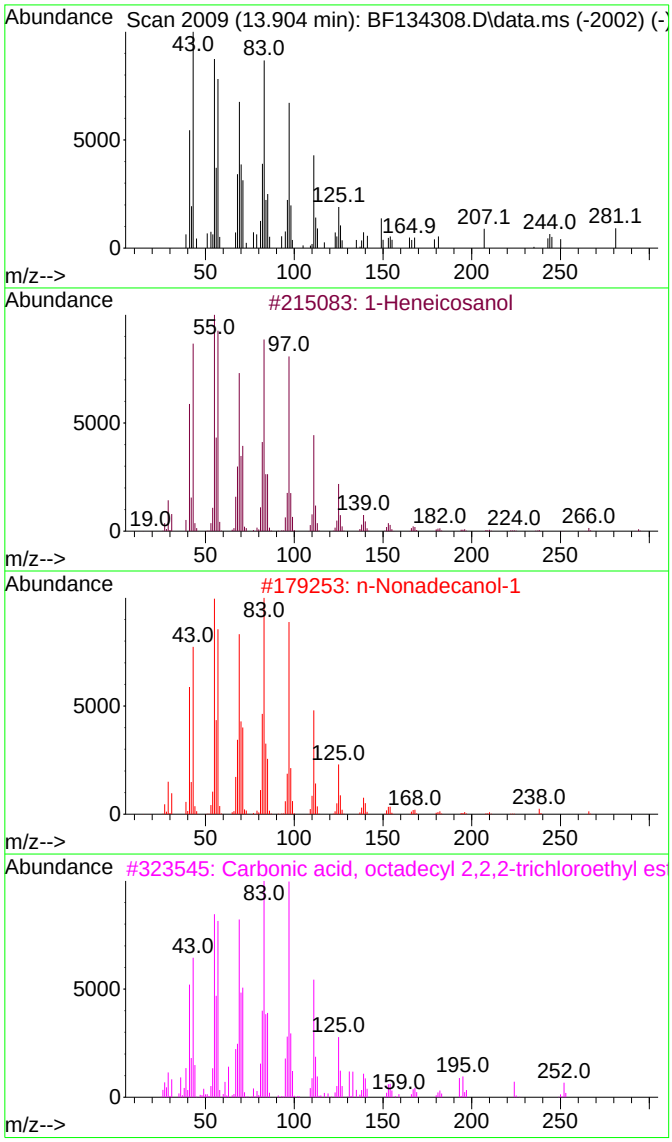
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

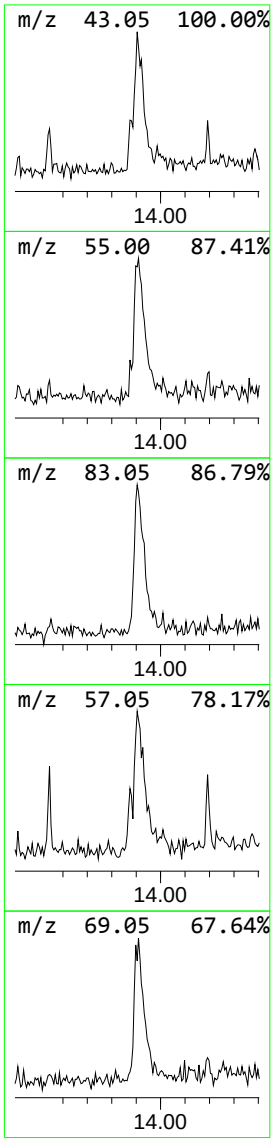
****

Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	4.53 ng	138559	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
3	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	93
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
5	Eicosyl methyl ether	312	C21H44O	1000406-29-4	90





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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-44-(2-5)

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

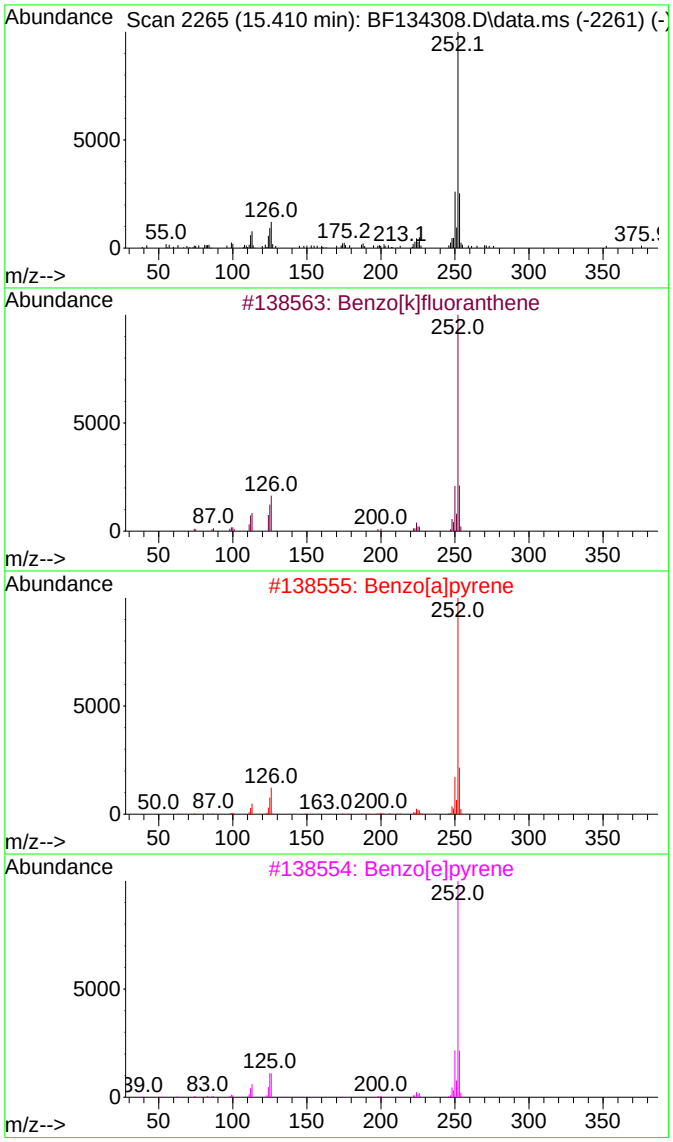
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

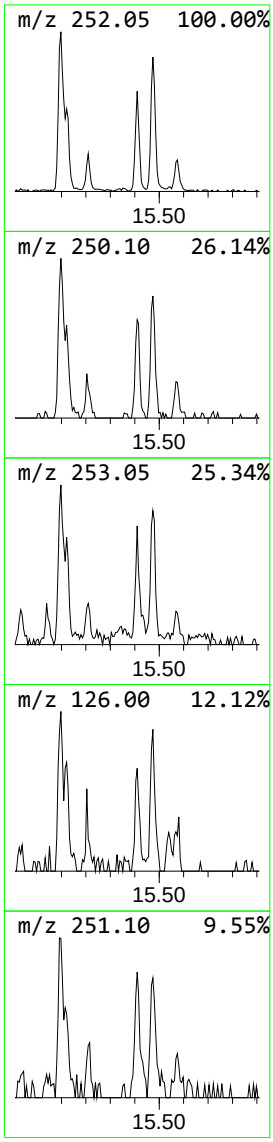
****

Peak Number 6 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.410	2.85 ng	58040	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
2	Benzo[a]pyrene	252	C20H12	000050-32-8	94
3	Benzo[e]pyrene	252	C20H12	000192-97-2	94
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
5	Perylene	252	C20H12	000198-55-0	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071423\
Data File : BF134308.D
Acq On : 15 Jul 2023 01:30
Operator : CG\JU
Sample : 03597-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-44-(2-5)

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
Ethanol, 2-(2-e...	6.675	2.5	ng	61281	1	6.840	491591	20.0
2,4,7,9-Tetrame...	9.310	14.9	ng	485076	3	9.881	652466	20.0
n-Hexadecanoic ...	11.904	6.1	ng	189848	4	11.375	626206	20.0
10-Octadecenoic...	12.475	3.7	ng	117033	4	11.375	626206	20.0
1-Heneicosanol	13.904	4.5	ng	138559	5	14.033	611858	20.0
Benzo[e]pyrene	15.410	2.9	ng	58040	6	15.539	407108	20.0