LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131176.D
Acq On : 12 Nov 2022 03:41
Operator : CG\JU
Sample : N5508-01 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-06-110722

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-BF110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131176.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	3	9	14	rVB	426346	531907	4.70%	1.782%
2	5.087	506	510	520	rBV	157498	166383	1.47%	0.558%
3	5.493	575	579	595	rVB	1056922	953728	8.43%	3.196%
4	6.504	747	751	761	rBV	1056298	938732	8.30%	3.146%
5	6.875	811	814	818	rBV	536771	426684	3.77%	1.430%
6	7.440	906	910	913	rBV	627968	500604	4.42%	1.677%
7	8.163	1029	1033	1036	rBV	598248	485373	4.29%	1.626%
8	9.234	1212	1215	1219	rVB	1009407	869278	7.68%	2.913%
9	9.922	1328	1332	1335	rBV	650920	493519	4.36%	1.654%
10	10.716	1463	1467	1470	rBV	500423	474995	4.20%	1.592%
11	11.416	1582	1586	1588	rBV	641993	517413	4.57%	1.734%
12	11.798	1647	1651	1655	rBV	2943133	2545185	22.49%	8.528%
13	11.945	1672	1676	1683	rBV	228327	247840	2.19%	0.830%
14	12.504	1764	1771	1773	rBV	7674613	11315380	100.00%	37.916%
15	12.527	1773	1775	1779	rVV2	6452561	5656088	49.99%	18.953%
16	12.598	1783	1787	1790	rVB	1764980	1463320	12.93%	4.903%
17	12.633	1790	1793	1796	rBV	170543	179941	1.59%	0.603%
18	13.004	1853	1856	1859	rBV	909510	774123	6.84%	2.594%
19	13.192	1884	1888	1891	rVB4	100037	138757	1.23%	0.465%
20	13.322	1907	1910	1915	rVB	158079	127828	1.13%	0.428%
21	13.992	2021	2024	2027	rVB	154469	134009	1.18%	0.449%
22	14.069	2033	2037	2040	rBV	414045	395428	3.49%	1.325%
23	14.163	2050	2053	2056	rVB	227815	211315	1.87%	0.708%
24	15.568	2288	2292	2297	rBV	227441	295519	2.61%	0.990%

Sum of corrected areas: 29843349

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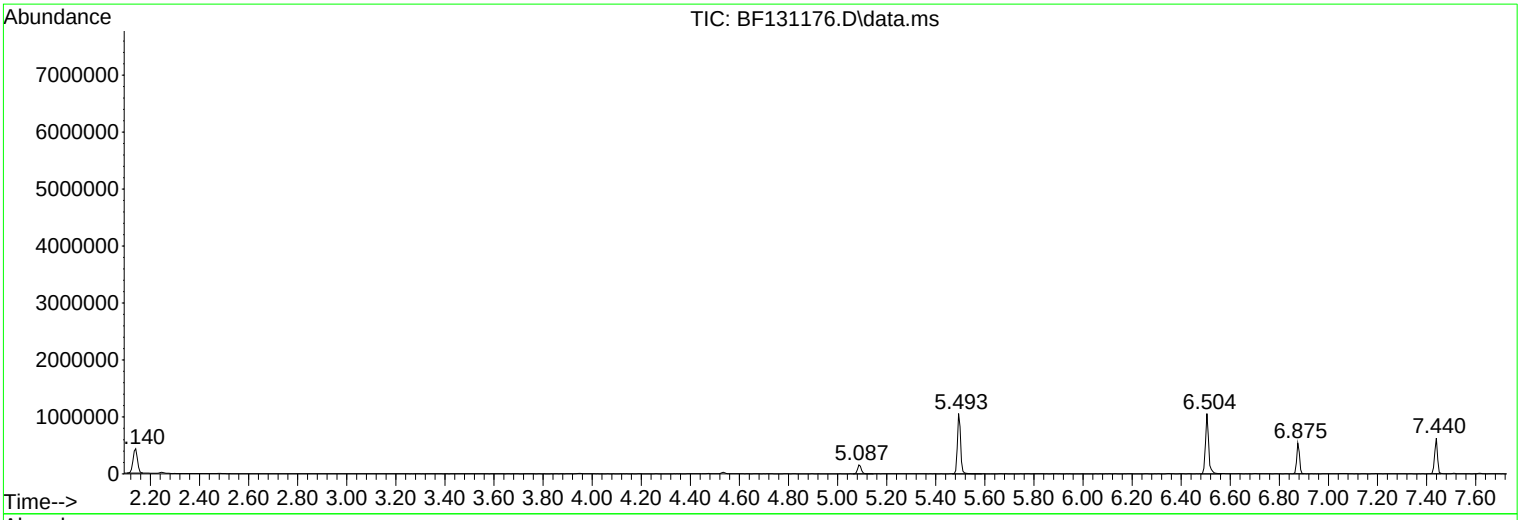
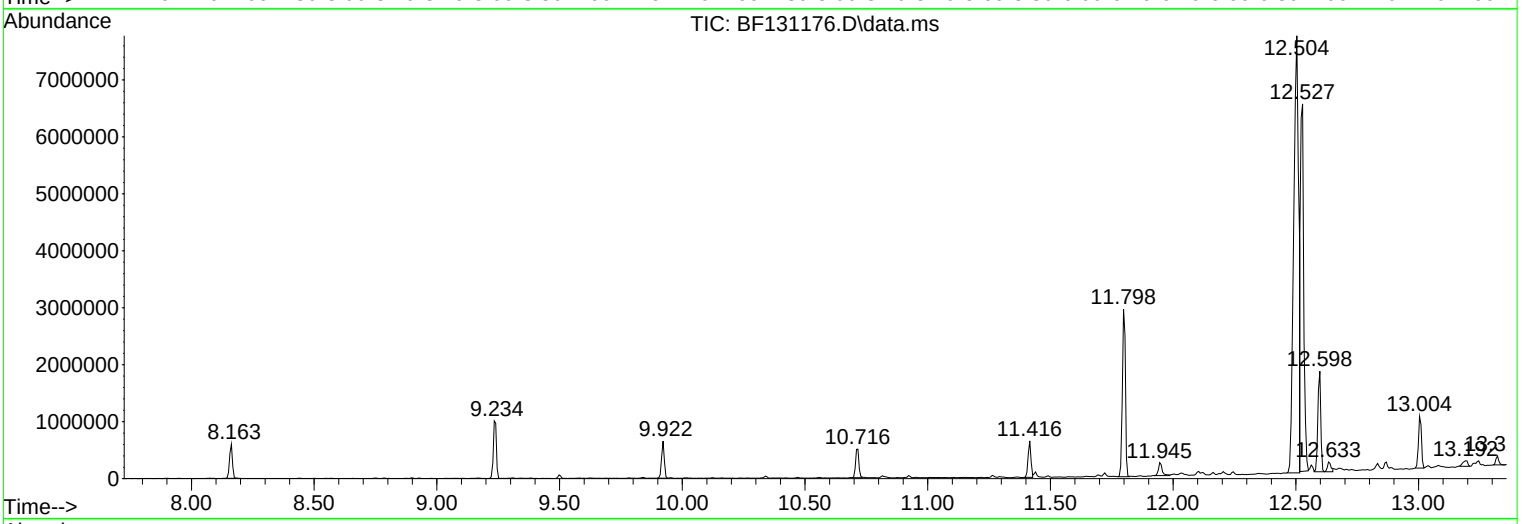
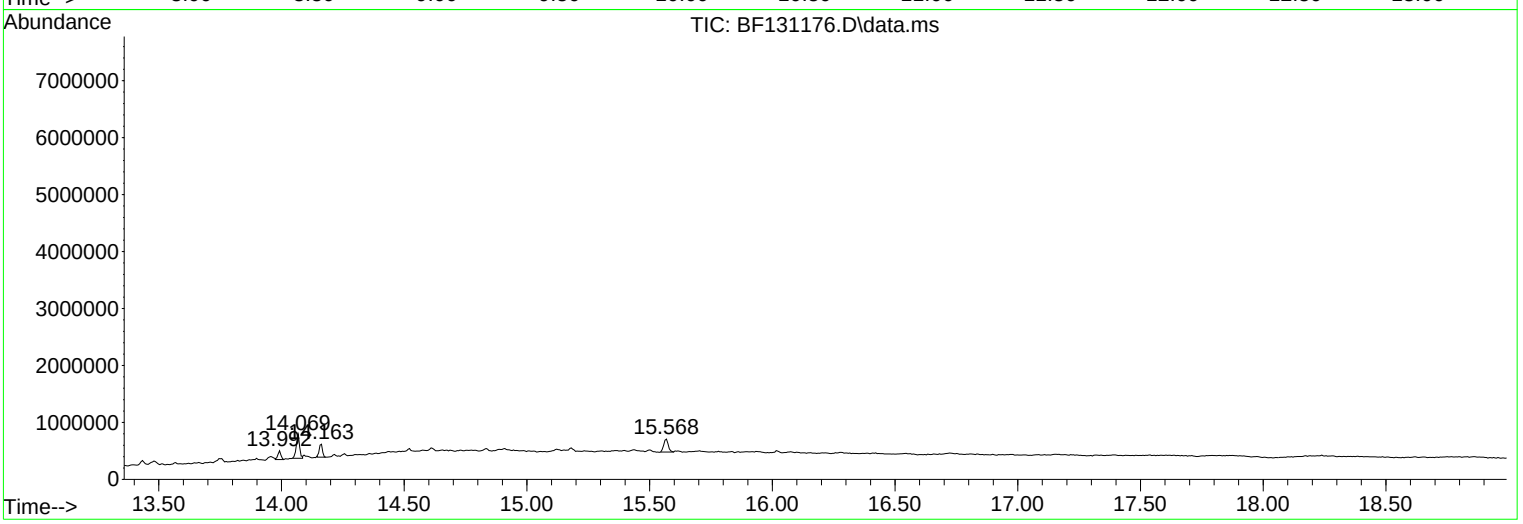
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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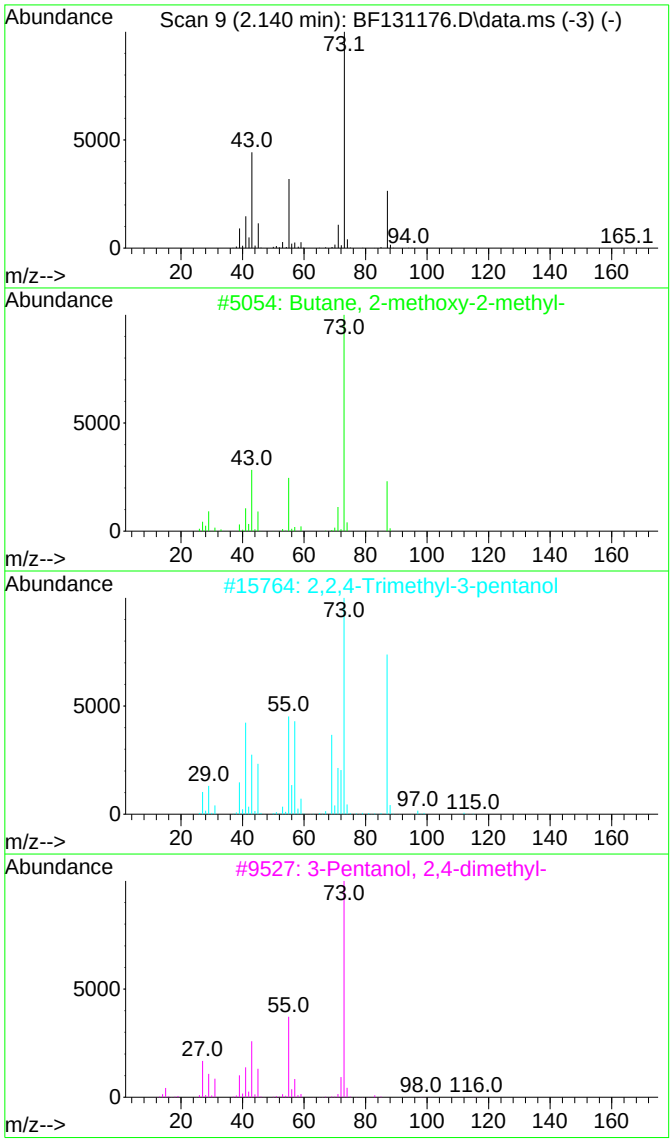
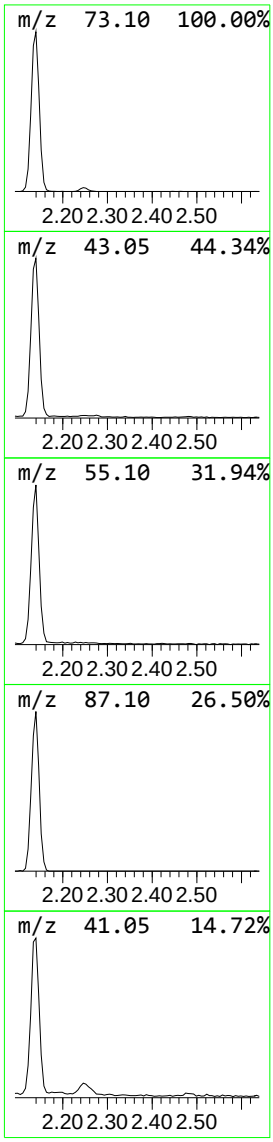
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	24.93 ng	531907	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
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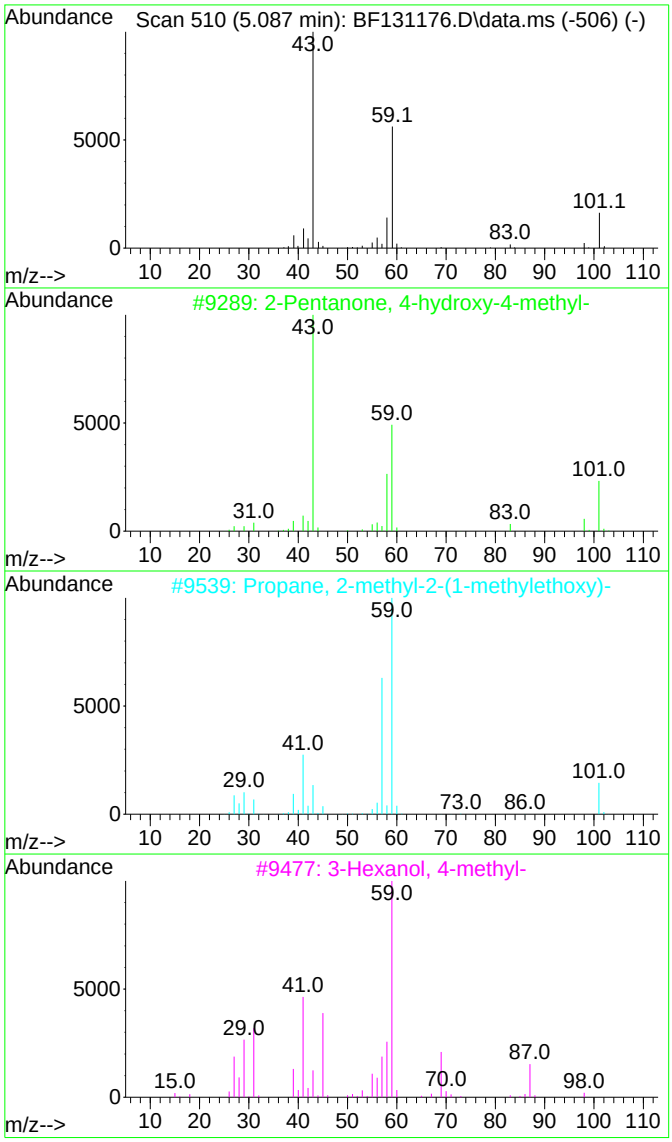
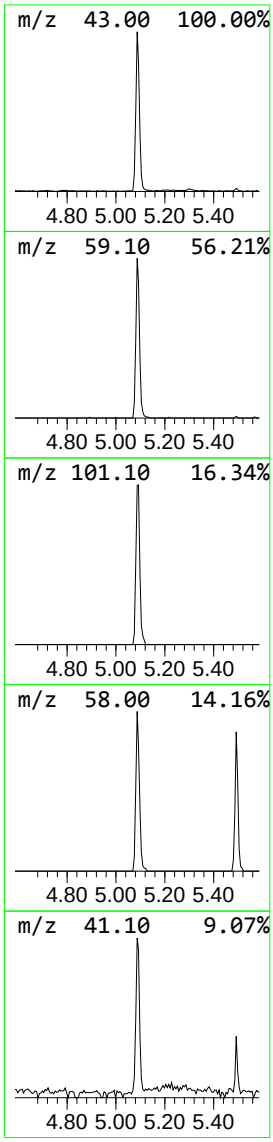
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	7.80 ng	166383	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27





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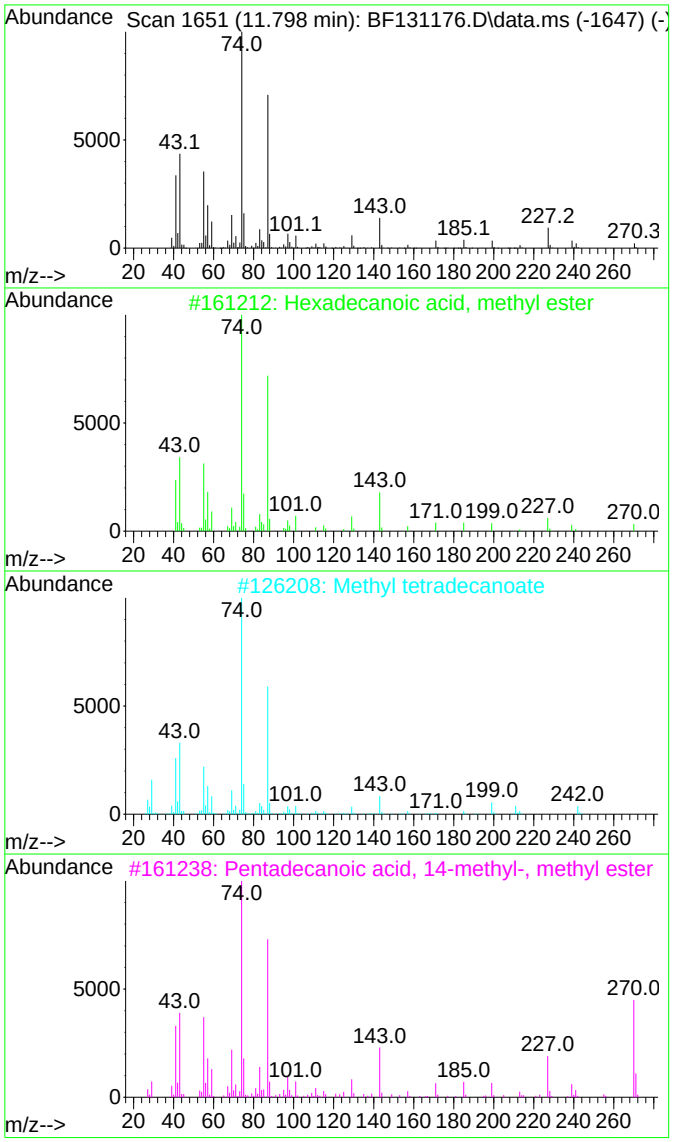
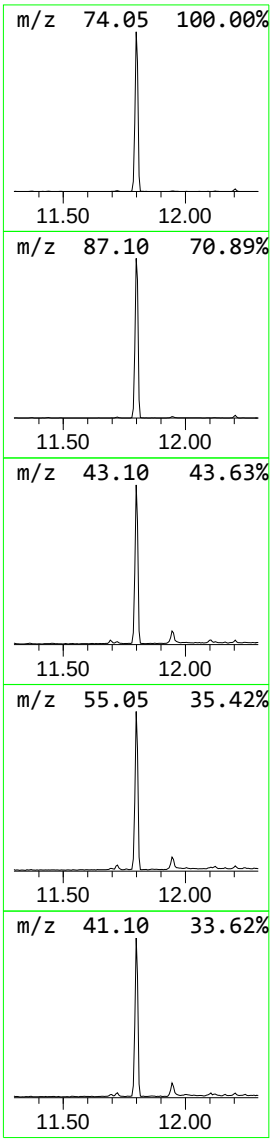
****
Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.798	98.38 ng	2545190	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2	Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	90
4	Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	87
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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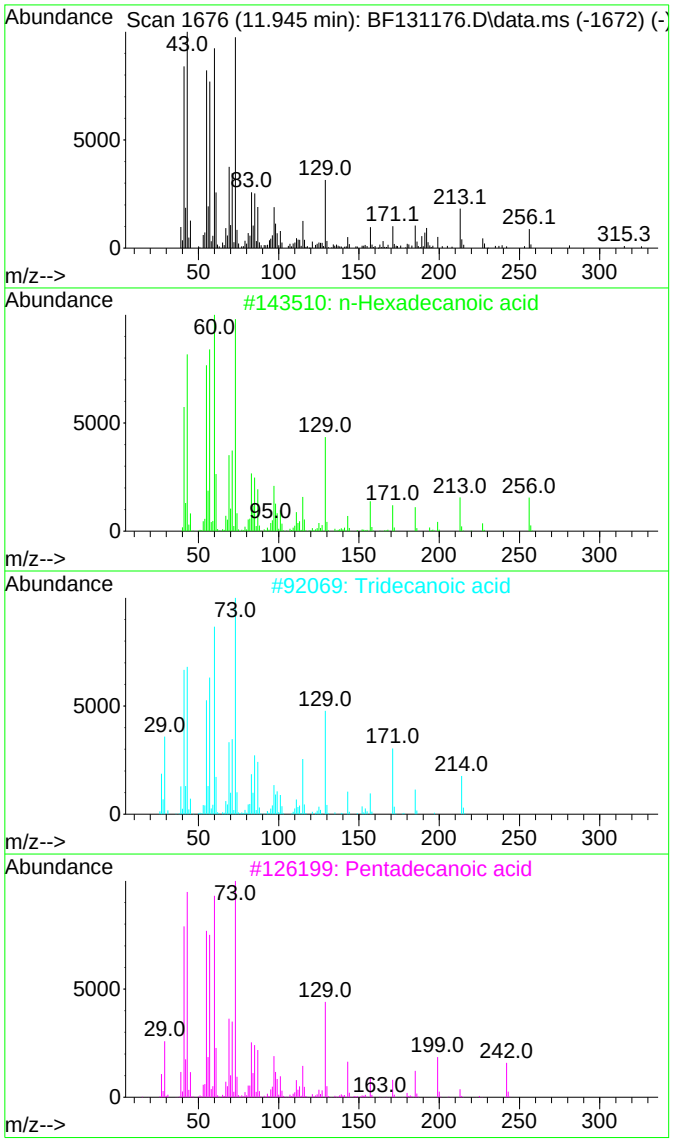
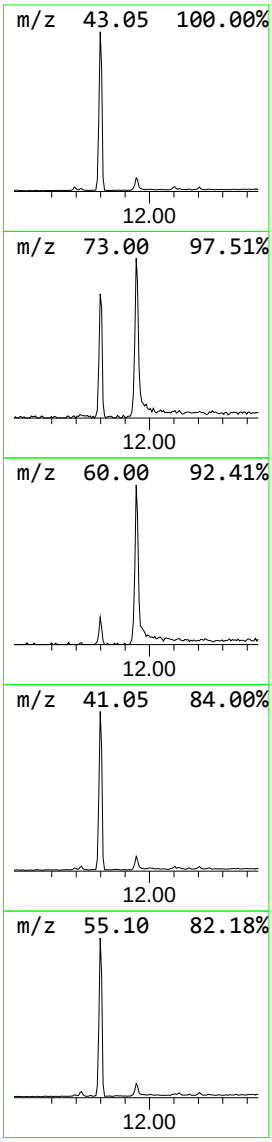
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	9.58 ng	247840	Phenanthrene-d10	11.416

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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5	Octadecanoic acid	284	C18H36O2	000057-11-4	60





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Instrument :
BNA_F
ClientSampleId :
AU-06-110722

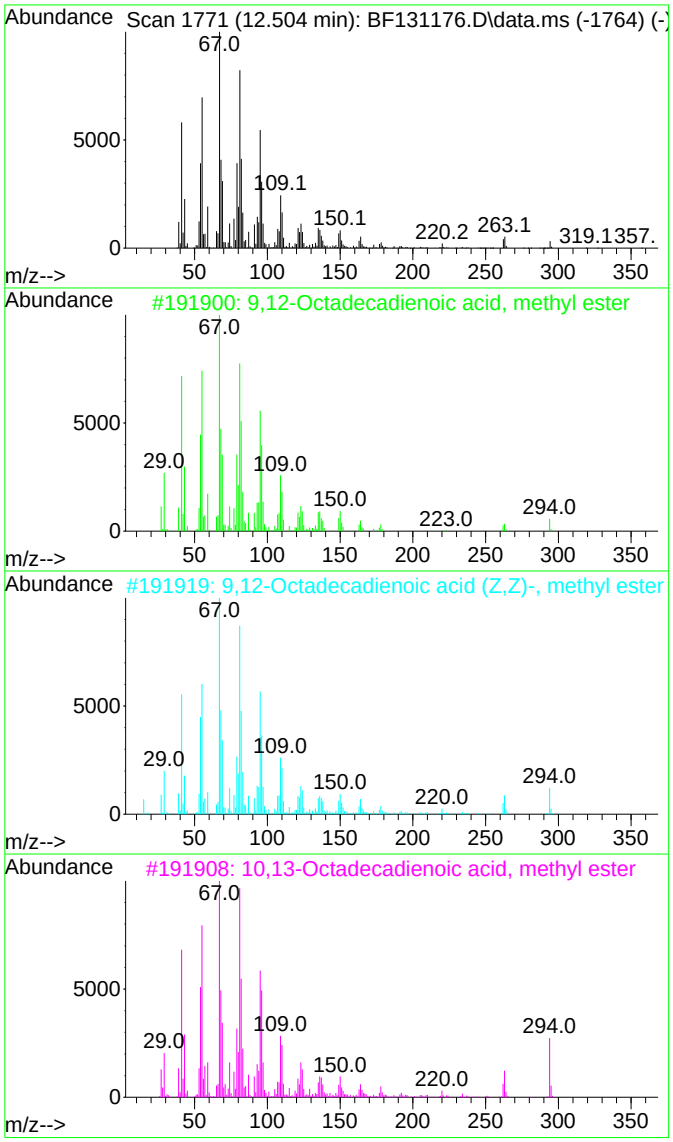
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

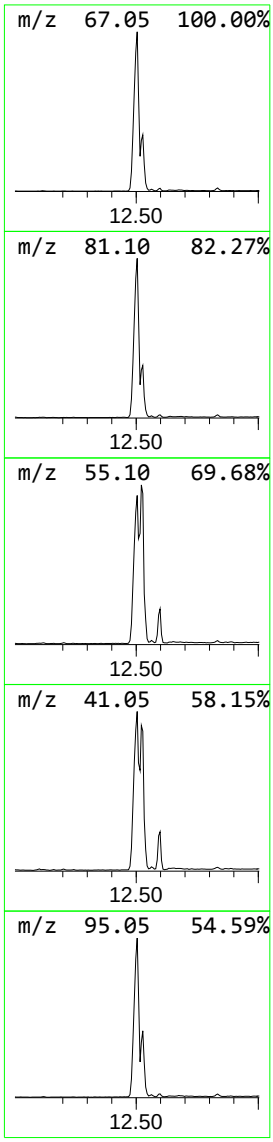
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.504	437.38 ng	11315400	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
3	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
5	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99





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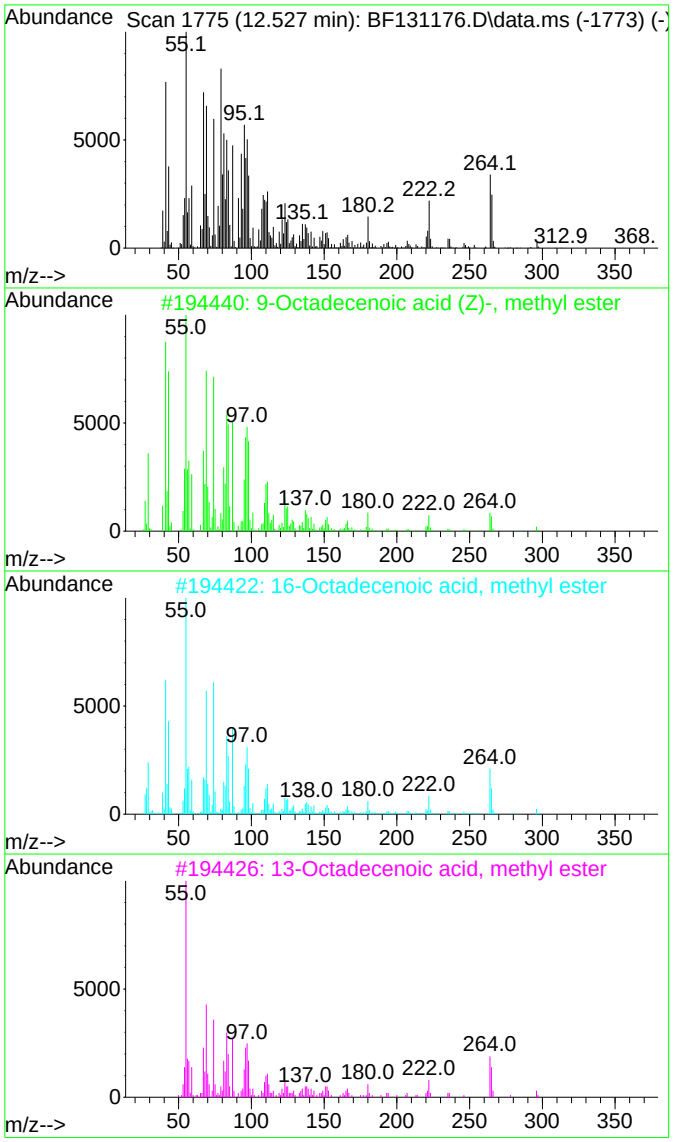
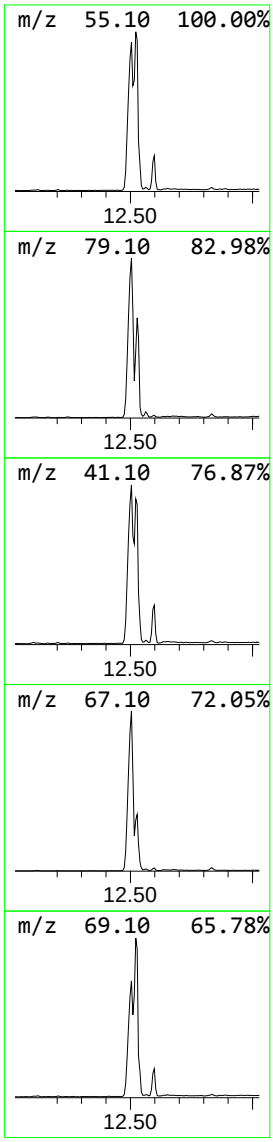
****

Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.527	218.63 ng	5656090	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	95
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	92
4	cis-10-Pentadecenoic acid, butyl...	296	C19H36O2	1000405-17-6	84
5	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	83





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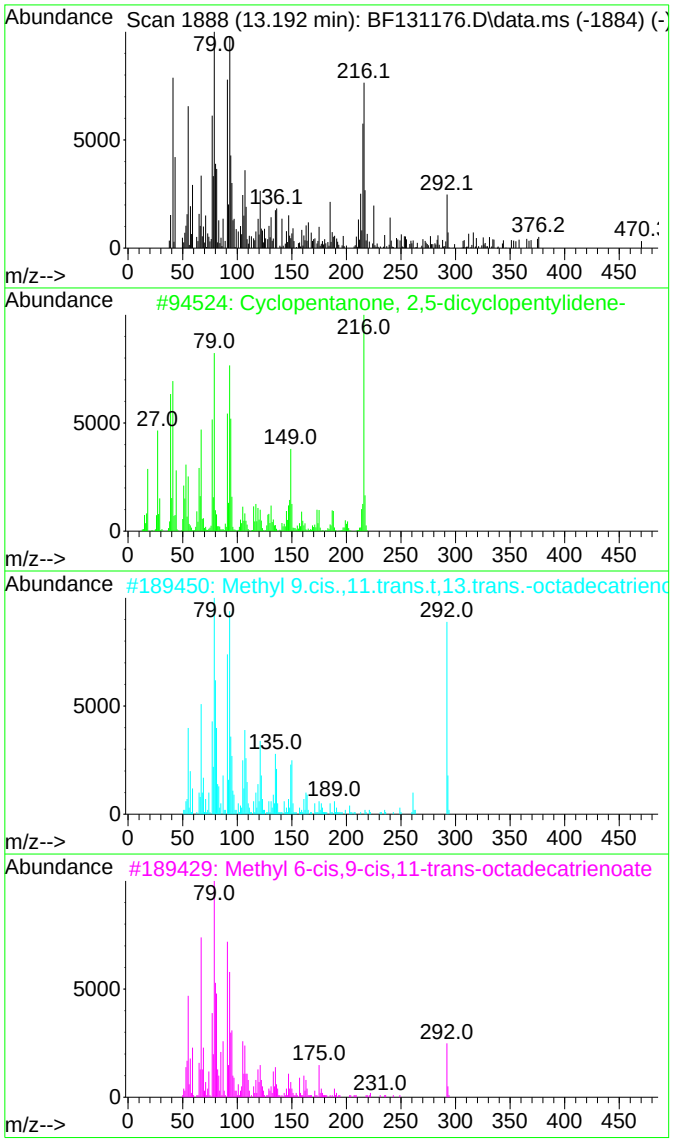
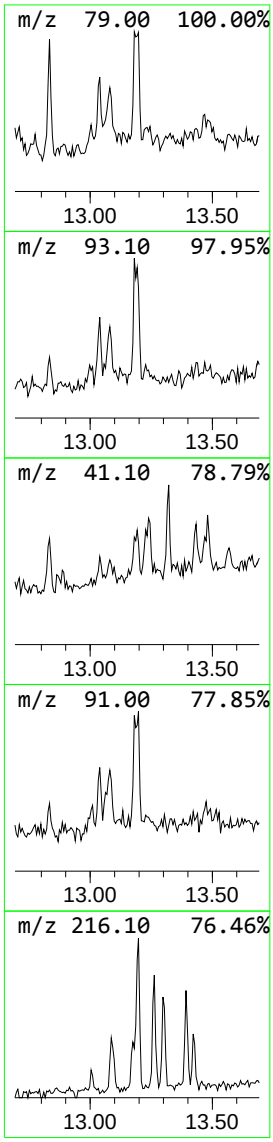
****

Peak Number 7 unknown13.192 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.192	7.02 ng	138757	Chrysene-d12	14.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone, 2,5-dicyclopenty...	216	C15H20O	005682-82-6	43
2	Methyl 9.cis.,11.trans.t,13.tran...	292	C19H32O2	1000336-42-6	43
3	Methyl 6-cis,9-cis,11-trans-octa...	292	C19H32O2	1010336-37-7	30
4	Bicyclo[3.2.1]oct-2-ene, 2-(phen...	216	C14H16S	1000142-98-5	25
5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	18





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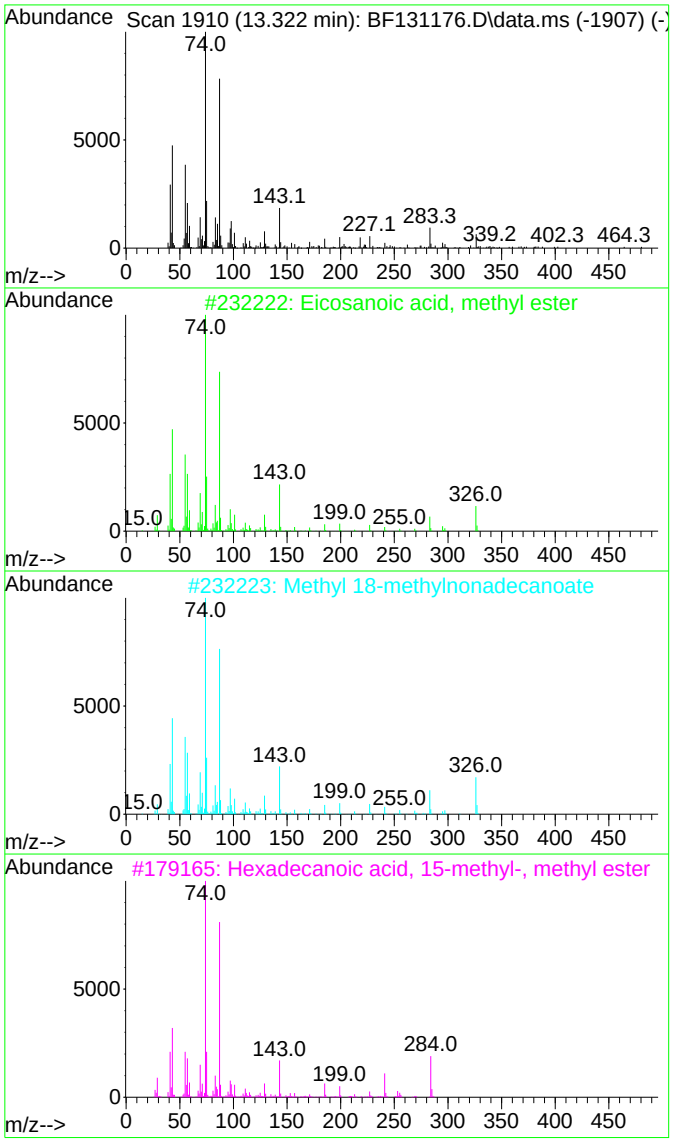
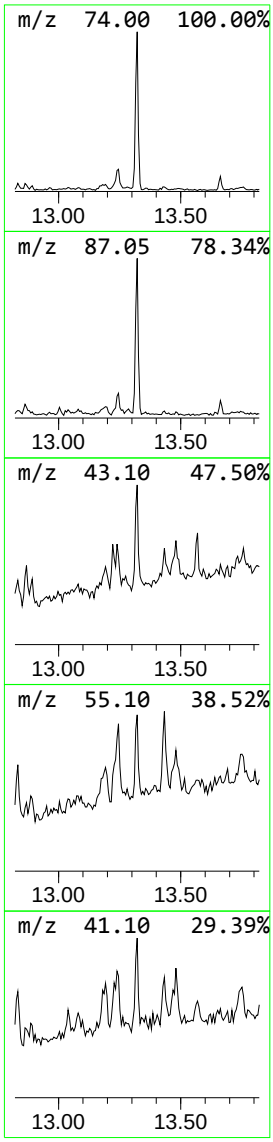
****
Peak Number 8 Eicosanoic acid, methyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.322	6.47 ng	127828	Chrysene-d12	14.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	95
2	Methyl 18-methylnonadecanoate	326	C21H42O2	1000424-52-4	94
3	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	91
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	87
5	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	83





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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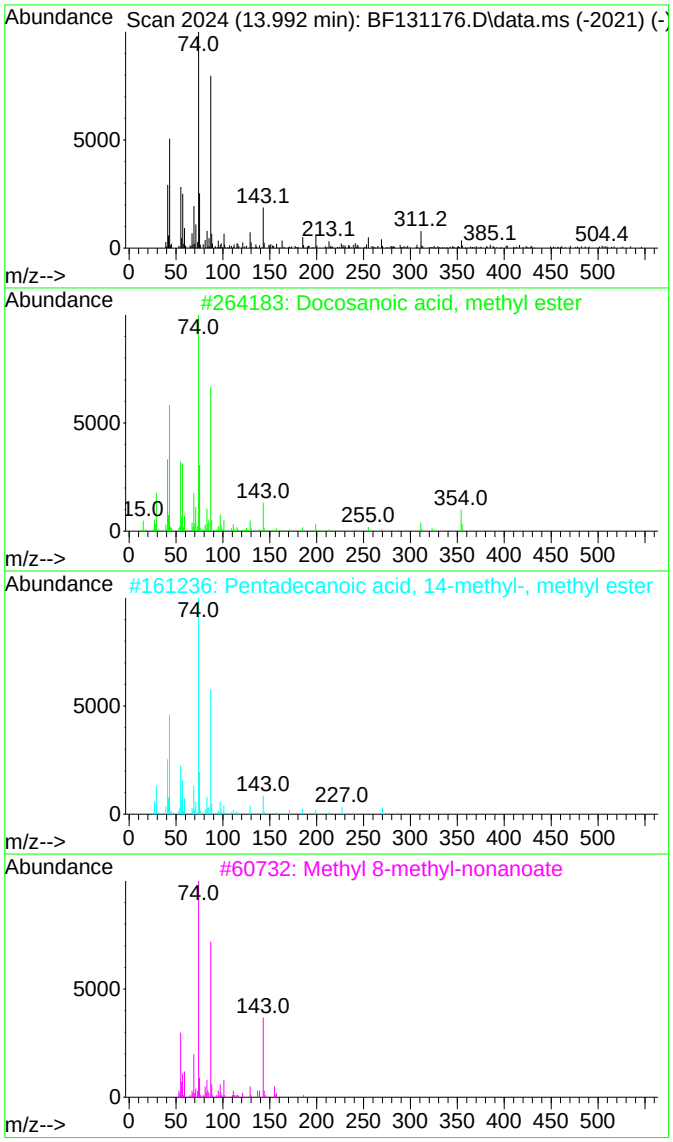
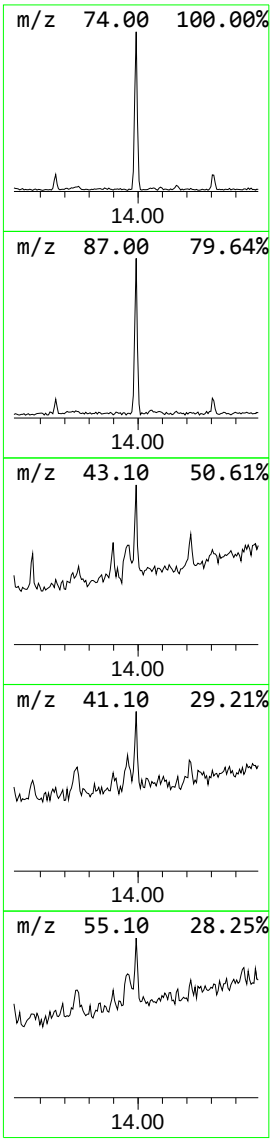
****
Peak Number 9 Docosanoic acid, methyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.992	6.78 ng	134009	Chrysene-d12	14.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	91
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87
3	Methyl 8-methyl-nonanoate	186	C11H22O2	1000452-00-9	83
4	Methyl stearate	298	C19H38O2	000112-61-8	80
5	Hexacosanoic acid, methyl ester	410	C27H54O2	005802-82-4	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131176.D
Acq On : 12 Nov 2022 03:41
Operator : CG\JU
Sample : N5508-01 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-06-110722

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

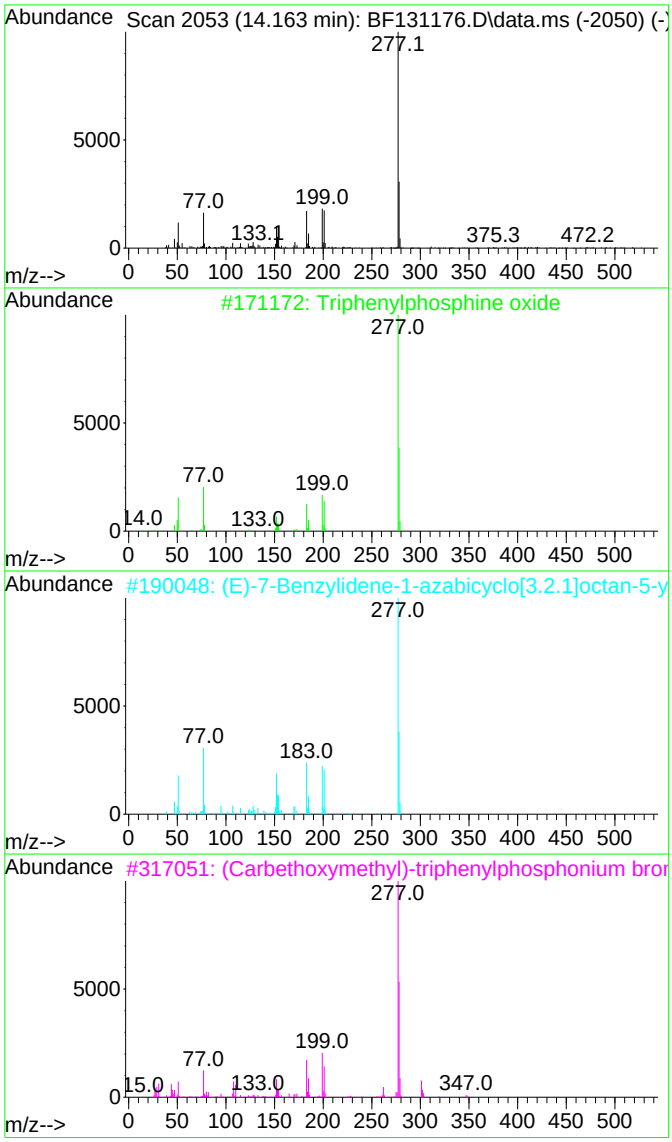
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

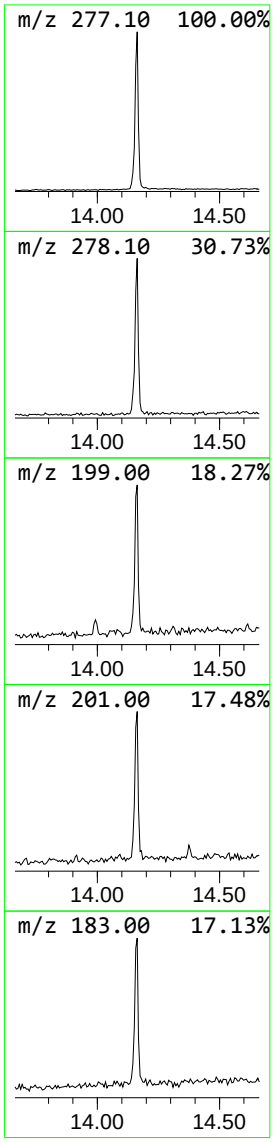
****

Peak Number 10 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.163	10.69 ng	211315	Chrysene-d12	14.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	86
3	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	40
4	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	37
5	5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	33





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131176.D
Acq On : 12 Nov 2022 03:41
Operator : CG\JU
Sample : N5508-01 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-06-110722

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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...	2.140	24.9	ng	531907	1	6.875	426684	20.0
2-Pentanone, 4-...	5.087	7.8	ng	166383	1	6.875	426684	20.0
Hexadecanoic ac...	11.798	98.4	ng	2545190	4	11.416	517413	20.0
n-Hexadecanoic ...	11.945	9.6	ng	247840	4	11.416	517413	20.0
9,12-Octadecadi...	12.504	437.4	ng	11315400	4	11.416	517413	20.0
9-Octadecenoic ...	12.527	218.6	ng	5656090	4	11.416	517413	20.0
unknown13.192	13.192	7.0	ng	138757	5	14.069	395428	20.0
Eicosanoic acid...	13.322	6.5	ng	127828	5	14.069	395428	20.0
Docosanoic acid...	13.992	6.8	ng	134009	5	14.069	395428	20.0
Triphenylphosph...	14.163	10.7	ng	211315	5	14.069	395428	20.0