LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
Data File : BF124199.D
Acq On : 9 Jun 2021 1:40
Operator : JU/CG
Sample : M2628-01 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-02-060721

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-BF060321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124199.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.492	576	579	587	rBV	185898	178775	23.72%	3.624%
2	6.510	748	752	759	rBV	157506	173695	23.05%	3.521%
3	6.863	809	812	815	rBV	297675	227443	30.18%	4.610%
4	7.422	904	907	912	rBV	134587	114789	15.23%	2.327%
5	8.145	1027	1030	1034	rVB	296702	254528	33.77%	5.159%
6	9.222	1210	1213	1218	rVB	233868	186963	24.81%	3.790%
7	9.298	1223	1226	1229	rBV	12775	11936	1.58%	0.242%
8	9.339	1229	1233	1237	rBV3	11512	11797	1.57%	0.239%
9	9.616	1277	1280	1283	rBV2	40746	40029	5.31%	0.811%
10	9.827	1312	1316	1321	rVB	21940	23507	3.12%	0.476%
11	9.904	1325	1329	1333	rVB	339291	266451	35.35%	5.401%
12	10.151	1369	1371	1375	rBV4	7861	11677	1.55%	0.237%
13	10.327	1395	1401	1404	rBV	27195	32012	4.25%	0.649%
14	10.551	1434	1439	1441	rBV2	18071	21218	2.82%	0.430%
15	10.692	1460	1463	1467	rBV	129497	105467	13.99%	2.138%
16	10.804	1478	1482	1483	rBV	42553	34349	4.56%	0.696%
17	11.251	1556	1558	1561	rBV	36530	26605	3.53%	0.539%
18	11.280	1561	1563	1569	rVB3	19691	22609	3.00%	0.458%
19	11.392	1579	1582	1585	rBV	322755	259014	34.37%	5.250%
20	11.416	1585	1586	1588	rVB	21594	11608	1.54%	0.235%
21	11.680	1629	1631	1633	rBV2	31824	23023	3.05%	0.467%
22	11.704	1633	1635	1637	rVB3	15849	9473	1.26%	0.192%
23	11.780	1644	1648	1651	rBV	299187	222659	29.54%	4.513%
24	11.892	1664	1667	1670	rBV4	8742	15274	2.03%	0.310%
25	11.921	1670	1672	1677	rVV6	14154	19780	2.62%	0.401%
26	12.027	1688	1690	1693	rVB3	15234	12962	1.72%	0.263%
27	12.086	1697	1700	1704	rVB4	25098	29819	3.96%	0.604%
28	12.186	1713	1717	1721	rBV5	7389	10237	1.36%	0.208%
29	12.445	1759	1761	1762	rBV2	18523	16517	2.19%	0.335%
30	12.468	1762	1765	1767	rVV	854242	720031	95.54%	14.595%
31	12.492	1767	1769	1775	rVB	901057	753662	100.00%	15.277%
32	12.574	1780	1783	1786	rVB	153250	120171	15.94%	2.436%
33	12.610	1786	1789	1792	rBV2	40885	40794	5.41%	0.827%
34	12.639	1792	1794	1796	rBV3	10283	12482	1.66%	0.253%
35	12.815	1820	1824	1825	rBV3	22445	25124	3.33%	0.509%
36	12.839	1825	1828	1835	rVB2	54294	75989	10.08%	1.540%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
Data File : BF124199.D
Acq On : 9 Jun 2021 1:40
Operator : JU/CG
Sample : M2628-01 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-02-060721

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-BF060321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.898	1835	1838	1840	rBV4	12685	14057	1.87%	0.285%
38	12.974	1848	1851	1856	rBV	245352	215599	28.61%	4.370%
39	13.057	1861	1865	1867	rBV4	17213	23394	3.10%	0.474%
40	13.133	1876	1878	1880	rBV3	25917	25551	3.39%	0.518%
41	13.204	1888	1890	1892	rBV3	25447	27009	3.58%	0.547%
42	13.268	1899	1901	1903	rBV3	21315	18667	2.48%	0.378%
43	13.298	1904	1906	1910	rVB4	23766	21765	2.89%	0.441%
44	13.427	1926	1928	1930	rBV3	16399	18133	2.41%	0.368%
45	13.515	1941	1943	1944	rBV2	15355	12599	1.67%	0.255%
46	13.545	1946	1948	1951	rVB4	22306	23764	3.15%	0.482%
47	14.039	2028	2032	2035	rBV	249386	236985	31.44%	4.804%
48	15.527	2282	2285	2289	rBV	146658	173436	23.01%	3.516%

Sum of corrected areas: 4933428

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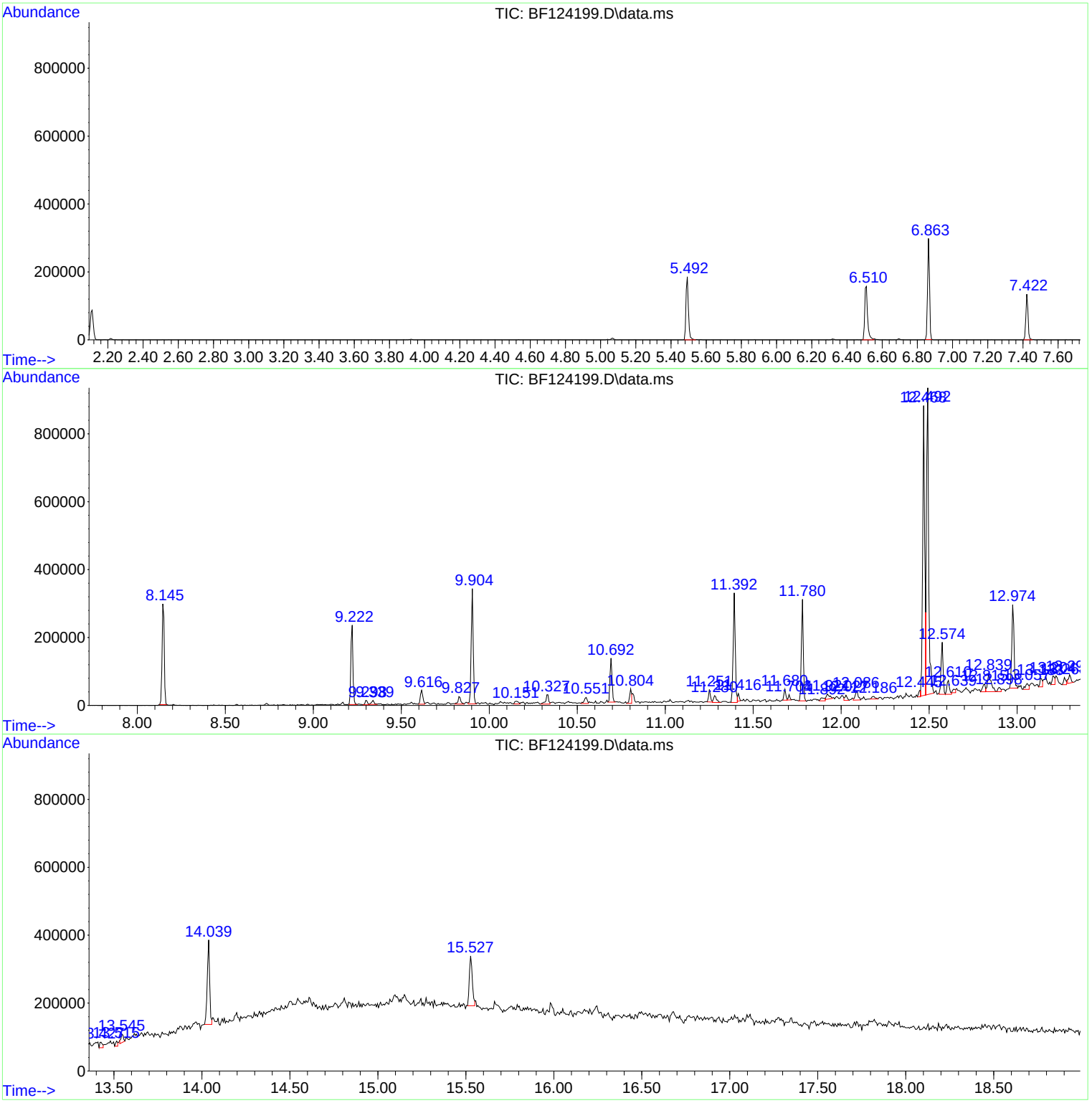
Instrument :
BNA_F
ClientSampleId :
HD-02-060721

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Data File : BF124199.D
Acq On : 9 Jun 2021 1:40
Operator : JU/CG
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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
HD-02-060721

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

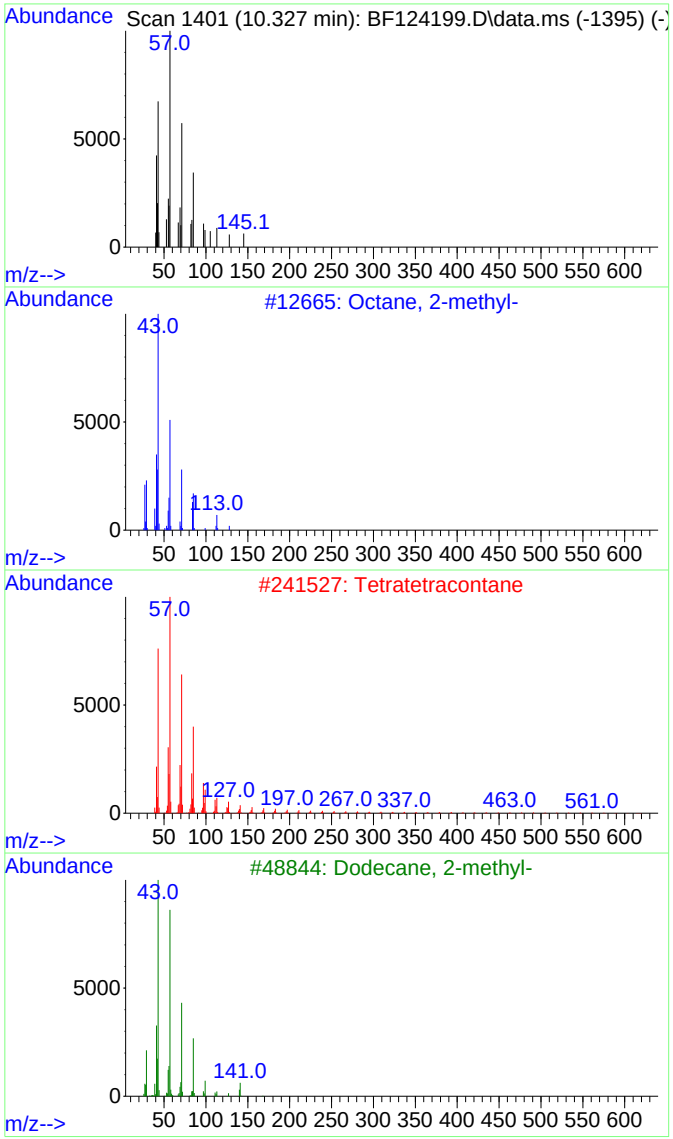
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

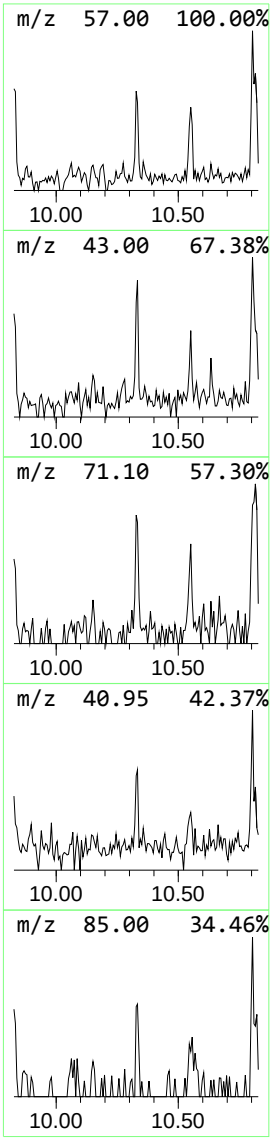
****

Peak Number 1 Octane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.327	2.40 ng	32012	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-methyl-	128	C9H20	003221-61-2	64
2	Tetratetracontane	619	C44H90	007098-22-8	64
3	Dodecane, 2-methyl-	184	C13H28	001560-97-0	64
4	Nonadecane	268	C19H40	000629-92-5	64
5	Decane, 2-methyl-	156	C11H24	006975-98-0	64





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Operator : JU/CG
Sample : M2628-01 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-060721

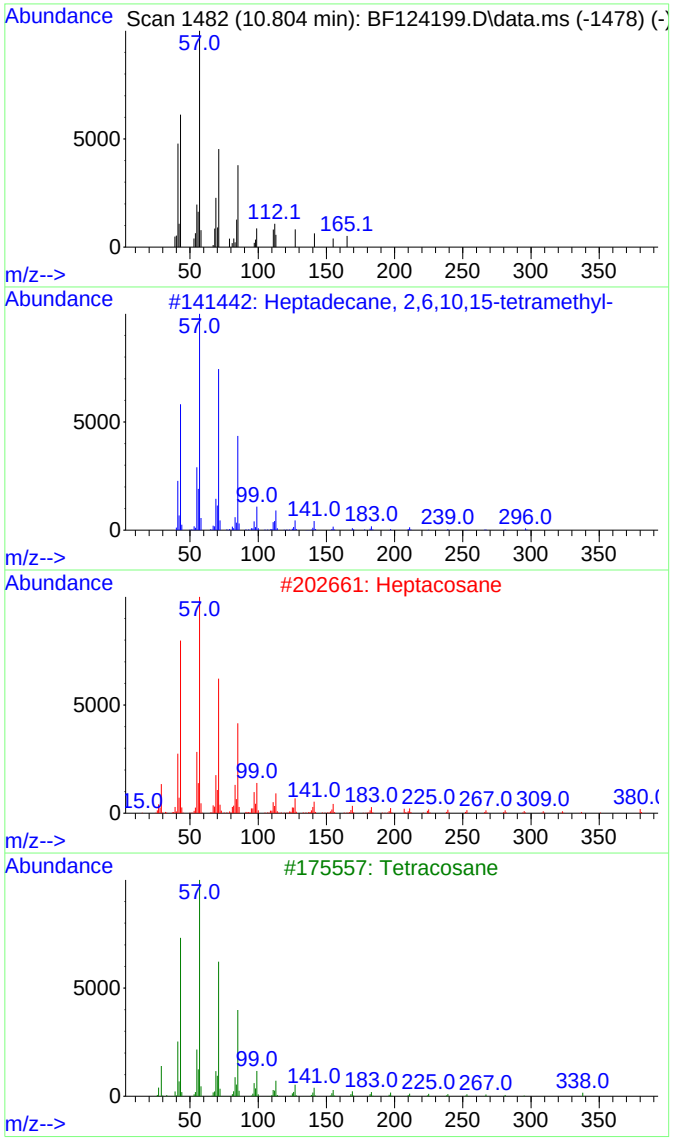
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

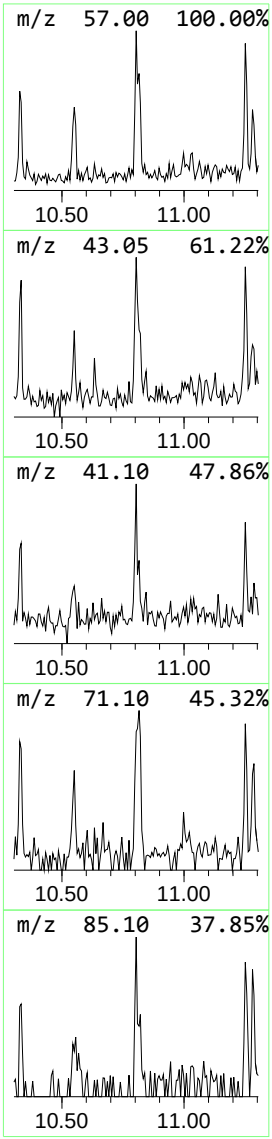
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Heptadecane, 2,6,10,15-tetr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.804	2.65 ng	34349	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	59
2	Heptacosane	380	C27H56	000593-49-7	59
3	Tetracosane	338	C24H50	000646-31-1	59
4	Pentadecane	212	C15H32	000629-62-9	59
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	59





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Acq On : 9 Jun 2021 1:40
Operator : JU/CG
Sample : M2628-01 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-02-060721

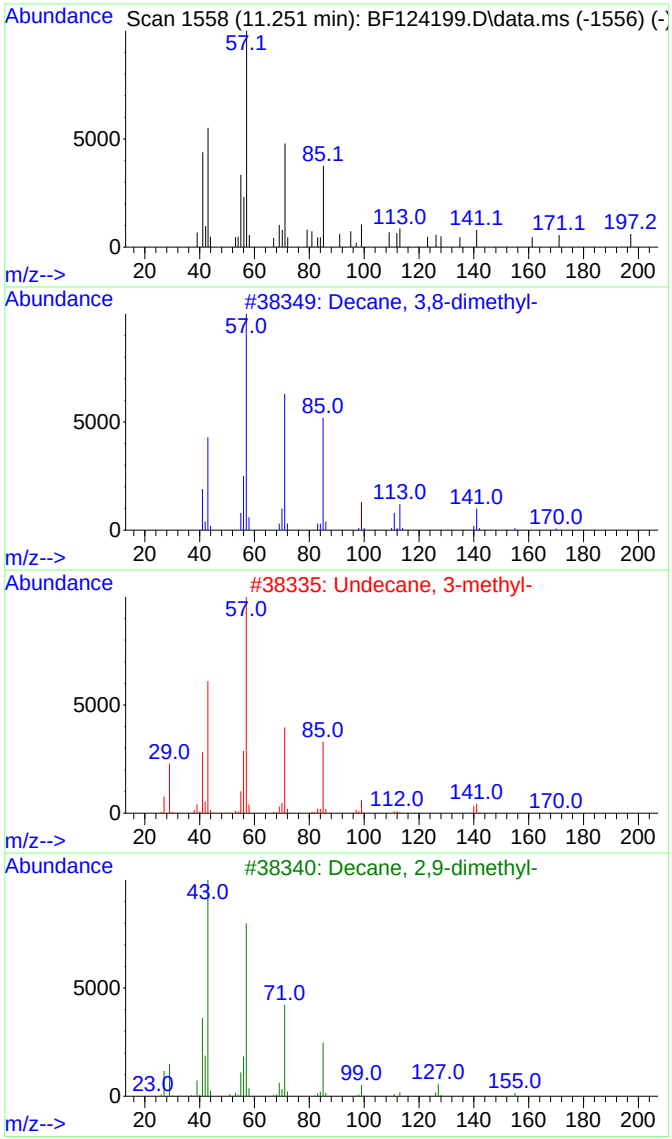
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

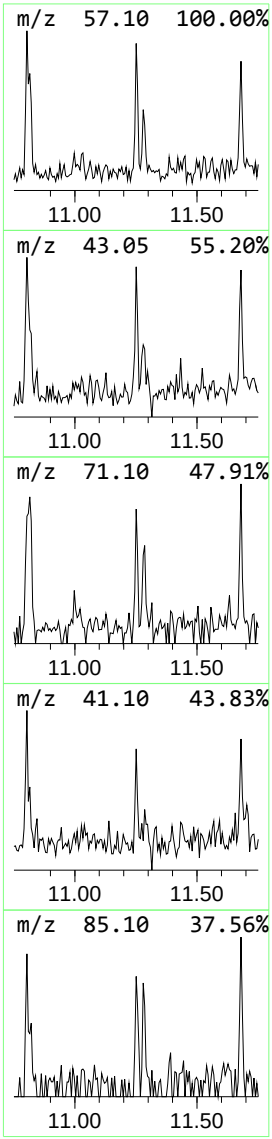
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Decane, 3,8-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.251	2.05 ng	26605	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	80
2	Undecane, 3-methyl-	170	C12H26	001002-43-3	72
3	Decane, 2,9-dimethyl-	170	C12H26	001002-17-1	64
4	Pentadecane	212	C15H32	000629-62-9	59
5	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	53





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Operator : JU/CG
Sample : M2628-01 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-060721

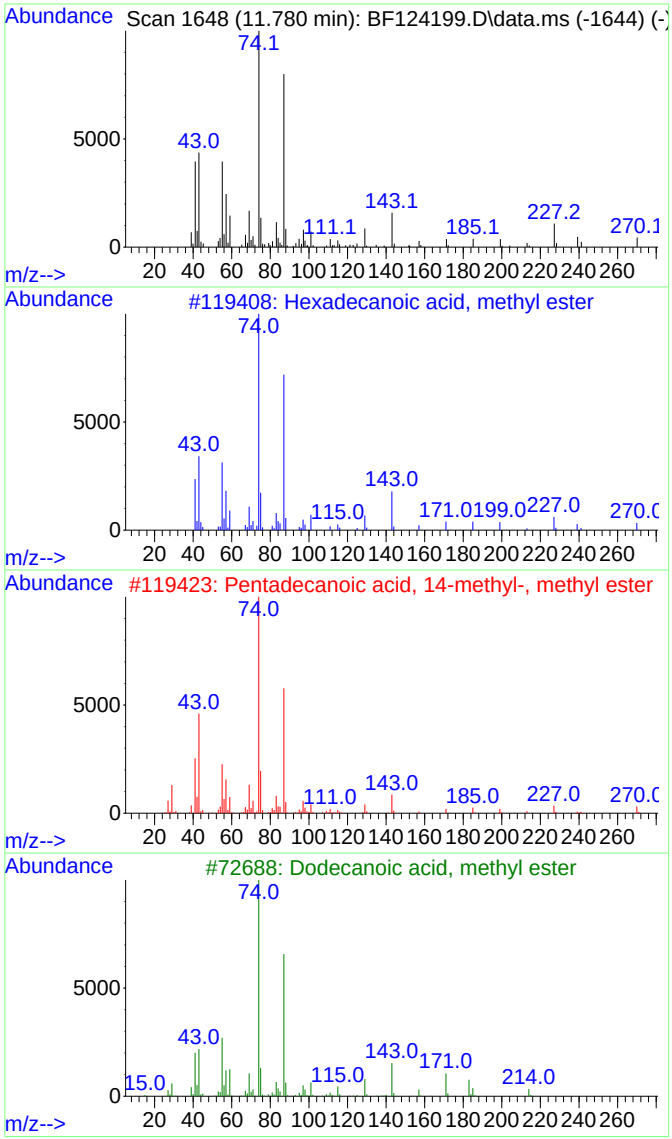
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

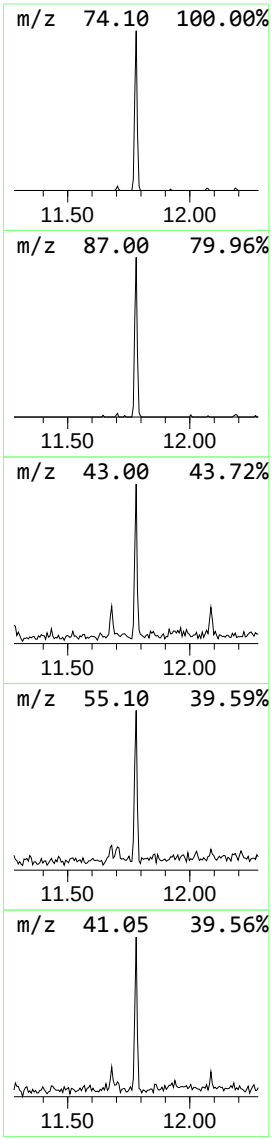
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.780	17.19 ng	222659	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	94
3	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	80
4	Undecanoic acid, 10-methyl-, met...	214	C13H26O2	005129-56-6	80
5	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	80





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Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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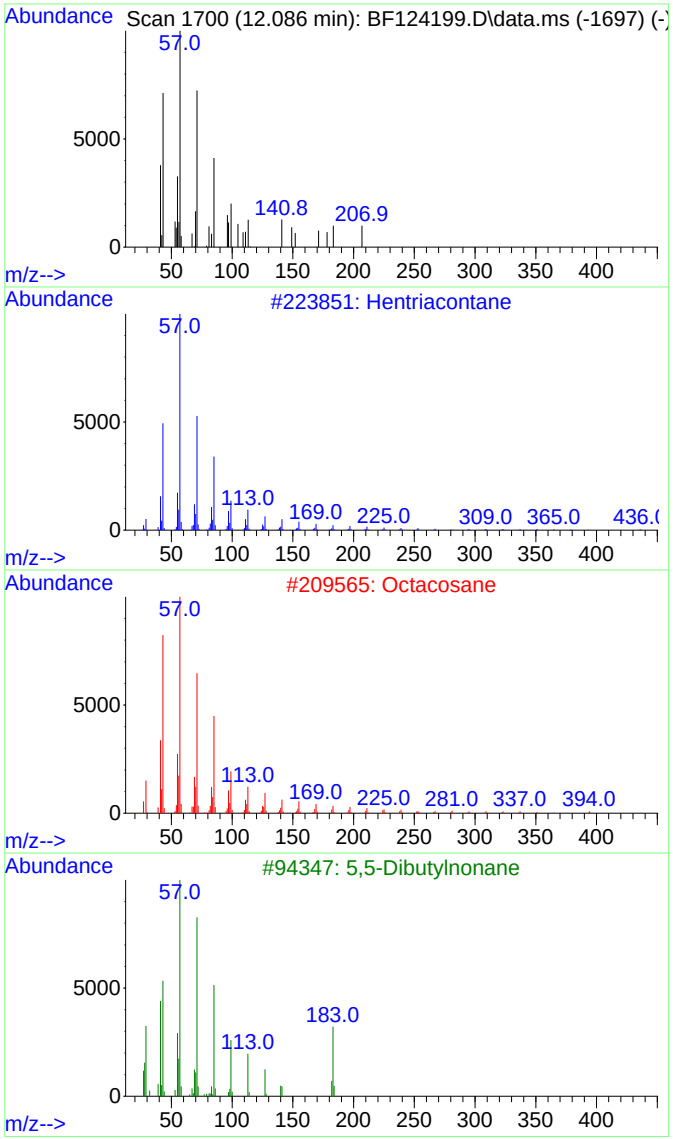
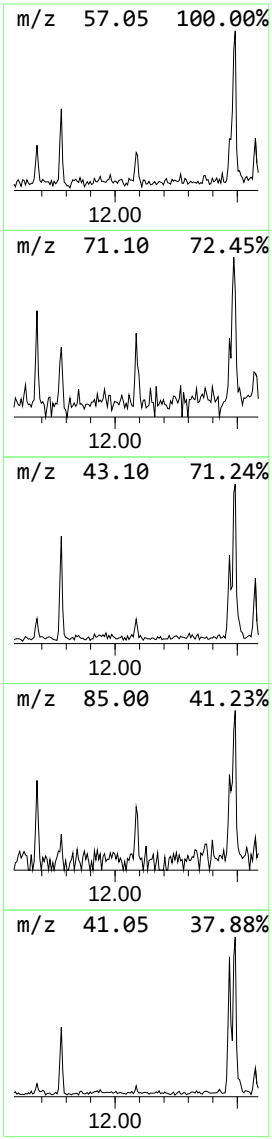
****

Peak Number 5 Hentriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.086	2.30 ng	29819	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	59
2	Octacosane	394	C28H58	000630-02-4	53
3	5,5-Dibutylnonane	240	C17H36	006008-17-9	53
4	Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	53
5	Heptadecane	240	C17H36	000629-78-7	53





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Operator : JU/CG
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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-060721

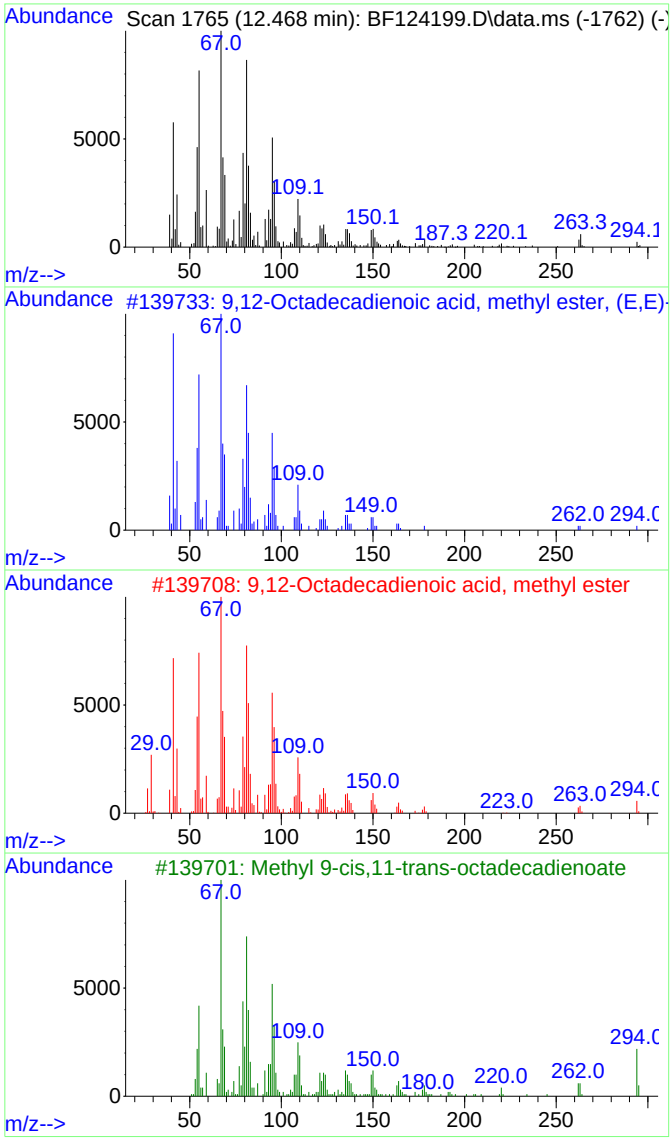
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

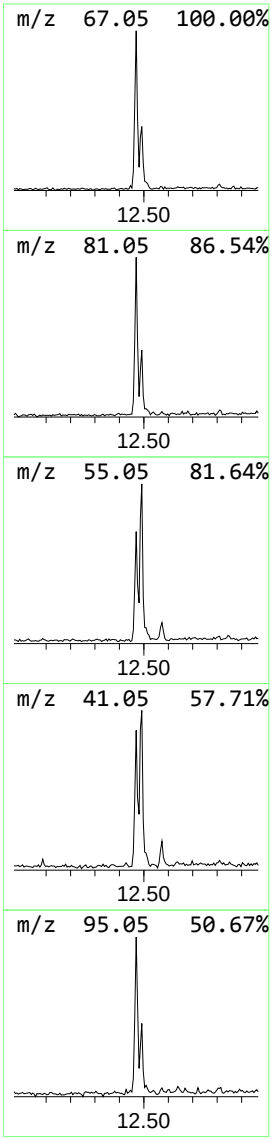
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.468	55.60 ng	720031	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	98
3	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	96
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	95
5	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	93





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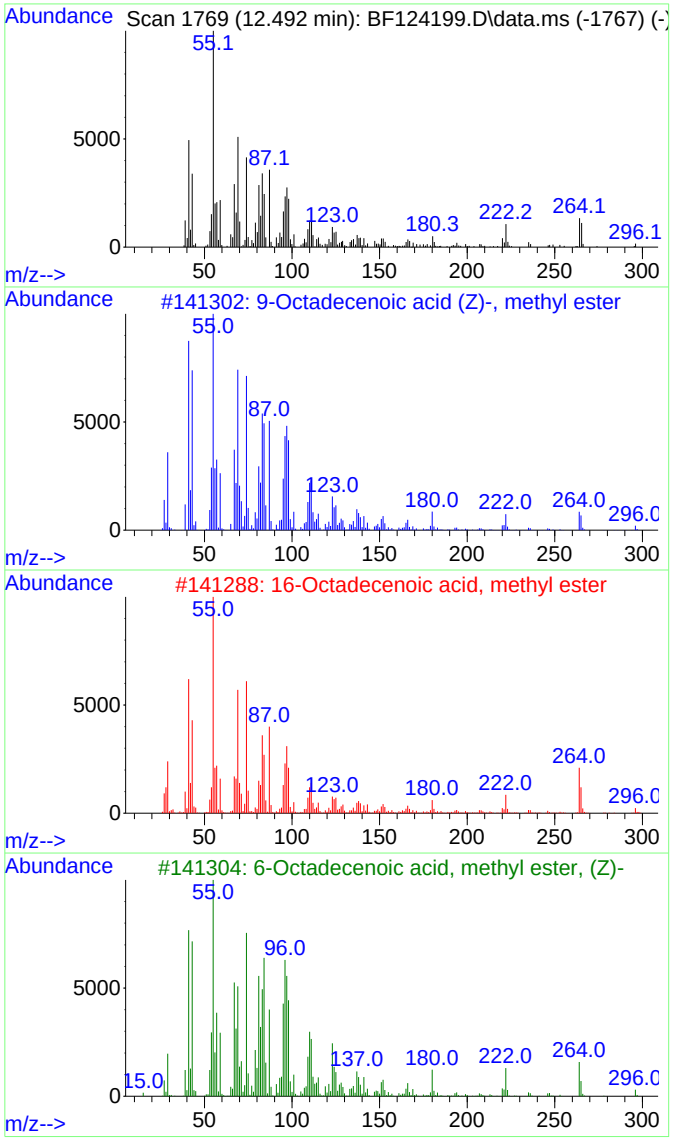
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

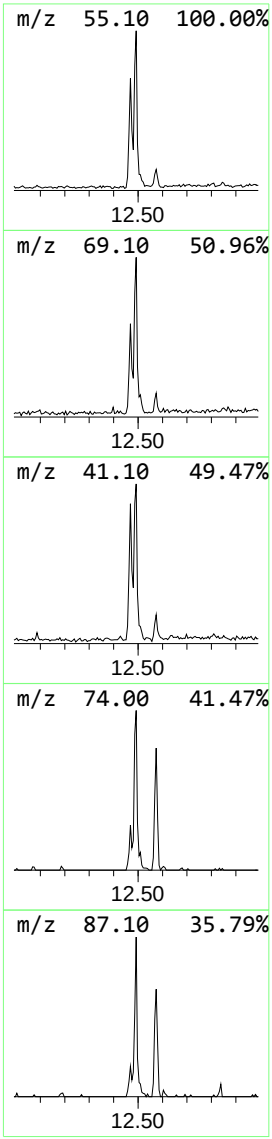
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 9-Octadecenoic acid (Z)-, m... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.492	58.19 ng	753662	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	98
2	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	98
3	6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	96
4	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	96
5	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	96





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Data File : BF124199.D
Acq On : 9 Jun 2021 1:40
Operator : JU/CG
Sample : M2628-01 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-060721

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

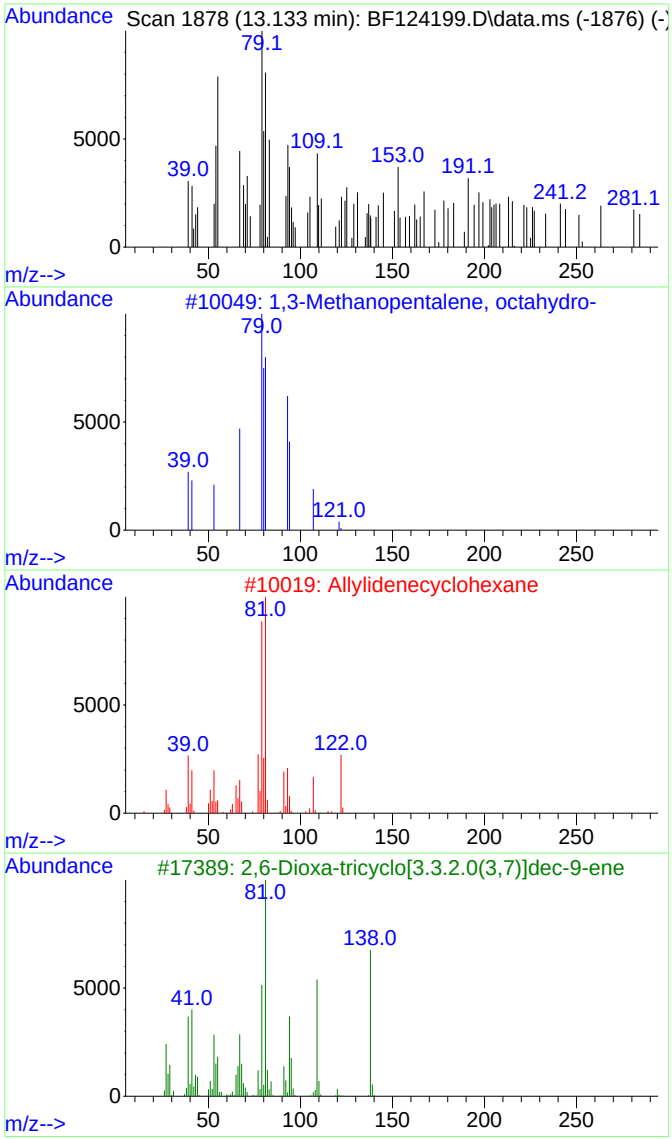
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

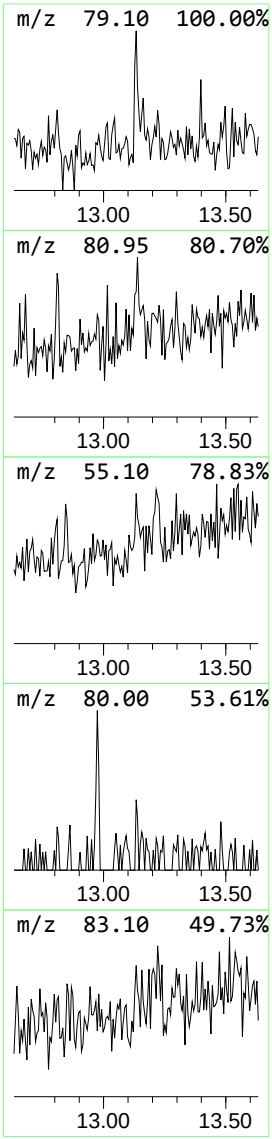
****

Peak Number 8 unknown13.133 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.133	2.16 ng	25551	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Methanopentalene, octahydro-	122	C9H14	013913-22-9	43
2	Allylidenecyclohexane	122	C9H14	005664-10-8	38
3	2,6-Dioxa-tricyclo[3.3.2.0(3,7)]...	138	C8H10O2	075568-75-1	35
4	Ethyl 3-cyclohexenecarboxylate	154	C9H14O2	015111-56-5	35
5	1-Cyclohexene-1-carboxylic acid	126	C7H10O2	000636-82-8	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
Data File : BF124199.D
Acq On : 9 Jun 2021 1:40
Operator : JU/CG
Sample : M2628-01 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-060721

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

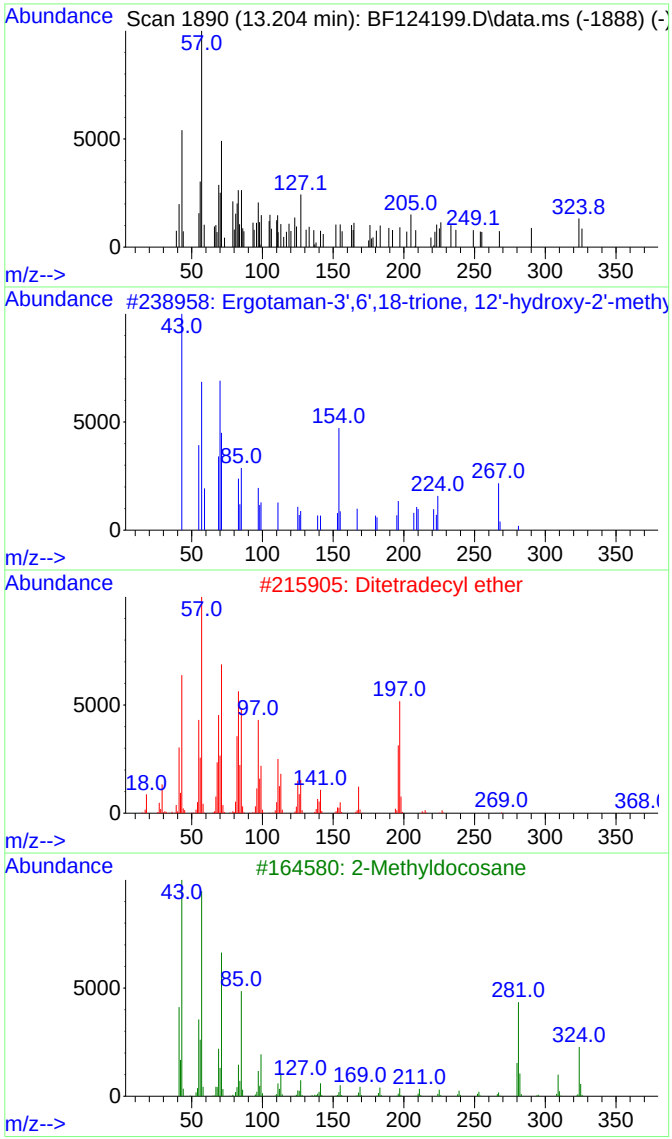
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

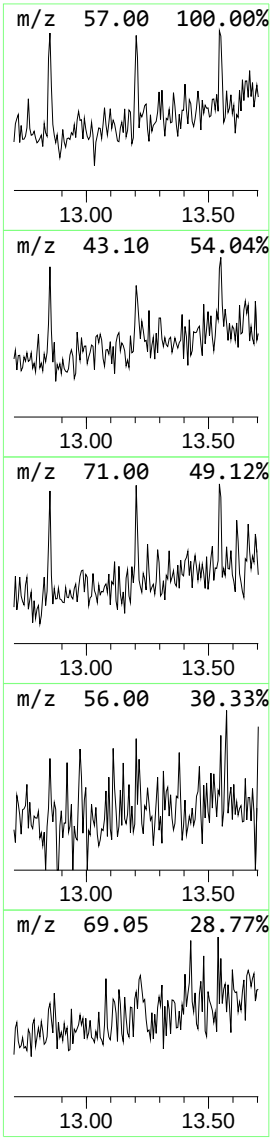
****

Peak Number 9 unknown13.204 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.204	2.28 ng	27009	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ergotaman-3',6',18-trione, 12'-h...	547	C30H37N5O5	000561-94-4	43
2	Ditetradecyl ether	410	C28H58O	005412-98-6	43
3	2-Methyldocosane	324	C23H48	001560-81-2	38
4	Octadecanoic acid, 2-propenyl ester	324	C21H40O2	006289-31-2	38
5	Tetradecanoic acid, 2-oxo-, meth...	256	C15H28O3	055682-82-1	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
Data File : BF124199.D
Acq On : 9 Jun 2021 1:40
Operator : JU/CG
Sample : M2628-01 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-02-060721

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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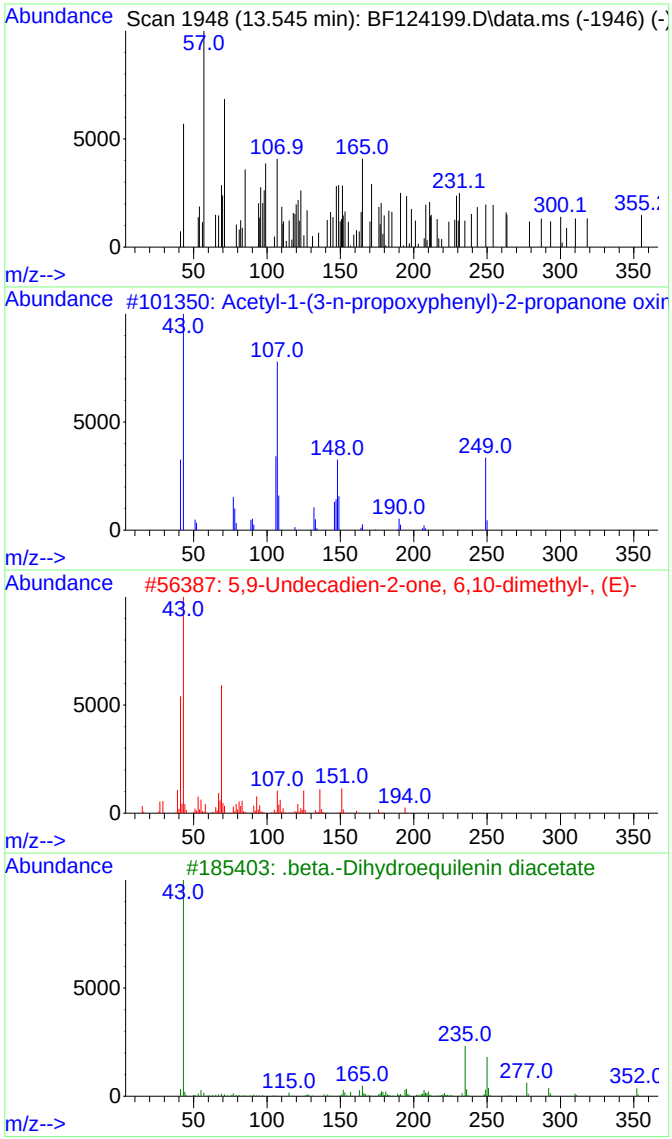
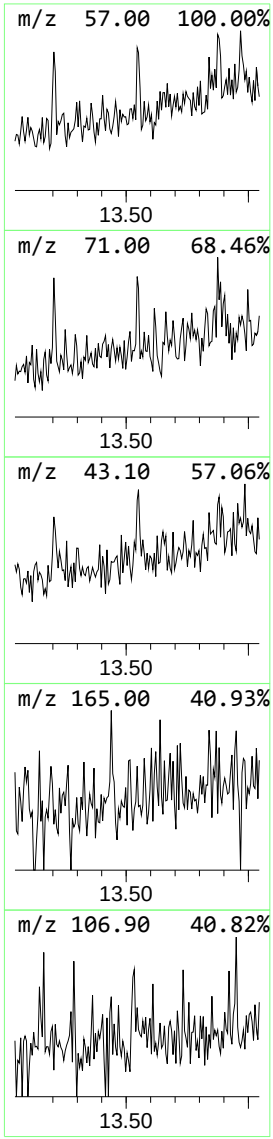
Peak Number 10 unknown13.545 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.545	2.01 ng	23764	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetyl-1-(3-n-propoxyphenyl)-2-p...	249	C14H19NO3	1000122-90-2	9
2	5,9-Undecadien-2-one, 6,10-dimet...	194	C13H22O	003796-70-1	9
3	.beta.-Dihydroequilenin diacetate	352	C22H24O4	001423-96-7	9
4	1-Heptadec-1-ynyl-cyclohexanol	334	C23H42O	1000296-77-9	9
5	2-Methyl-3-isobutoxy-5-propargyl...	206	C13H18O2	117780-93-5	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
Data File : BF124199.D
Acq On : 9 Jun 2021 1:40
Operator : JU/CG
Sample : M2628-01 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-02-060721

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Octane, 2-methyl-	10.327	2.4	ng	32012	3	9.904	266451	20.0
Heptadecane, 2,...	10.804	2.6	ng	34349	4	11.392	259014	20.0
Decane, 3,8-dim...	11.251	2.0	ng	26605	4	11.392	259014	20.0
Hexadecanoic ac...	11.780	17.2	ng	222659	4	11.392	259014	20.0
Hentriacontane	12.086	2.3	ng	29819	4	11.392	259014	20.0
9,12-Octadecadi...	12.468	55.6	ng	720031	4	11.392	259014	20.0
9-Octadecenoic ...	12.492	58.2	ng	753662	4	11.392	259014	20.0
unknown13.133	13.133	2.2	ng	25551	5	14.039	236985	20.0
unknown13.204	13.204	2.3	ng	27009	5	14.039	236985	20.0
unknown13.545	13.545	2.0	ng	23764	5	14.039	236985	20.0