LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052621\
Data File : BF124066.D
Acq On : 26 May 2021 15:43
Operator : JU/CG
Sample : M2517-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : METRO-SP

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-BF051421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124066.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	9	15	23	rVB	488188	598998	37.22%	4.586%
2	2.281	29	33	38	rVB2	32782	42365	2.63%	0.324%
3	5.110	509	514	521	rVB	410278	483264	30.03%	3.700%
4	5.516	578	583	586	rBV	1193653	1186291	73.71%	9.082%
5	5.904	646	649	655	rVB	43875	35086	2.18%	0.269%
6	6.516	748	753	756	rBV	1213272	1218141	75.69%	9.326%
7	6.722	784	788	801	rBV	19835	33811	2.10%	0.259%
8	6.893	813	817	820	rBV	441273	348374	21.65%	2.667%
9	7.451	907	912	915	rBV	936090	845028	52.51%	6.469%
10	8.175	1031	1035	1038	rBV	557139	439858	27.33%	3.368%
11	9.251	1213	1218	1221	rBV	2013794	1609351	100.00%	12.321%
12	9.363	1233	1237	1245	rVB	26941	31486	1.96%	0.241%
13	9.639	1281	1284	1289	rBV	81258	73315	4.56%	0.561%
14	9.933	1330	1334	1343	rVB	608771	554279	34.44%	4.244%
15	10.722	1464	1468	1471	rBV	1302788	1120001	69.59%	8.575%
16	10.845	1484	1489	1495	rVB2	30564	38485	2.39%	0.295%
17	11.316	1565	1569	1572	rBV	22552	23475	1.46%	0.180%
18	11.422	1583	1587	1589	rBV	669107	576182	35.80%	4.411%
19	11.445	1589	1591	1594	rVB	74574	59790	3.72%	0.458%
20	11.945	1674	1676	1683	rVB3	83864	72719	4.52%	0.557%
21	12.033	1688	1691	1693	rBV2	26562	24750	1.54%	0.189%
22	12.469	1762	1765	1769	rBV5	16187	21890	1.36%	0.168%
23	12.504	1769	1771	1778	rVB5	22035	26667	1.66%	0.204%
24	12.633	1790	1793	1796	rVB	161453	127438	7.92%	0.976%
25	12.863	1827	1832	1837	rVB	132829	135420	8.41%	1.037%
26	13.010	1849	1857	1860	rBV	1807397	1581807	98.29%	12.110%
27	13.080	1865	1869	1873	rBV7	14548	23602	1.47%	0.181%
28	13.298	1903	1906	1910	rVB4	29136	32638	2.03%	0.250%
29	13.698	1972	1974	1976	rBV3	22716	21434	1.33%	0.164%
30	13.951	2012	2017	2029	rVB10	79549	216238	13.44%	1.656%
31	14.063	2031	2036	2039	rVV2	401289	418928	26.03%	3.207%
32	14.086	2039	2040	2043	rVB	47926	36791	2.29%	0.282%
33	14.533	2113	2116	2120	rBV5	17302	23874	1.48%	0.183%
34	14.698	2140	2144	2146	rBV5	21082	30066	1.87%	0.230%
35	14.845	2167	2169	2173	rVB5	20763	21514	1.34%	0.165%
36	14.921	2178	2182	2186	rBV2	51282	62070	3.86%	0.475%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052621\
Data File : BF124066.D
Acq On : 26 May 2021 15:43
Operator : JU/CG
Sample : M2517-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : METRO-SP

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-BF051421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.121	2211	2216	2224	rVB	60552	126139	7.84%	0.966%
38	15.192	2226	2228	2231	rVB	27027	25830	1.60%	0.198%
39	15.427	2265	2268	2275	rVB2	32145	45550	2.83%	0.349%
40	15.492	2275	2279	2284	rBV	45095	58784	3.65%	0.450%
41	15.557	2285	2290	2299	rVB	271891	394705	24.53%	3.022%
42	16.033	2368	2371	2378	rVB3	30102	47066	2.92%	0.360%
43	16.851	2507	2510	2516	rBV7	11144	23684	1.47%	0.181%
44	17.057	2539	2545	2551	rBV8	27284	53253	3.31%	0.408%
45	17.174	2561	2565	2570	rVB8	16300	27668	1.72%	0.212%
46	17.504	2617	2621	2622	rBV4	17133	22347	1.39%	0.171%
47	18.256	2742	2749	2753	rBV10	19743	41310	2.57%	0.316%

Sum of corrected areas: 13061762

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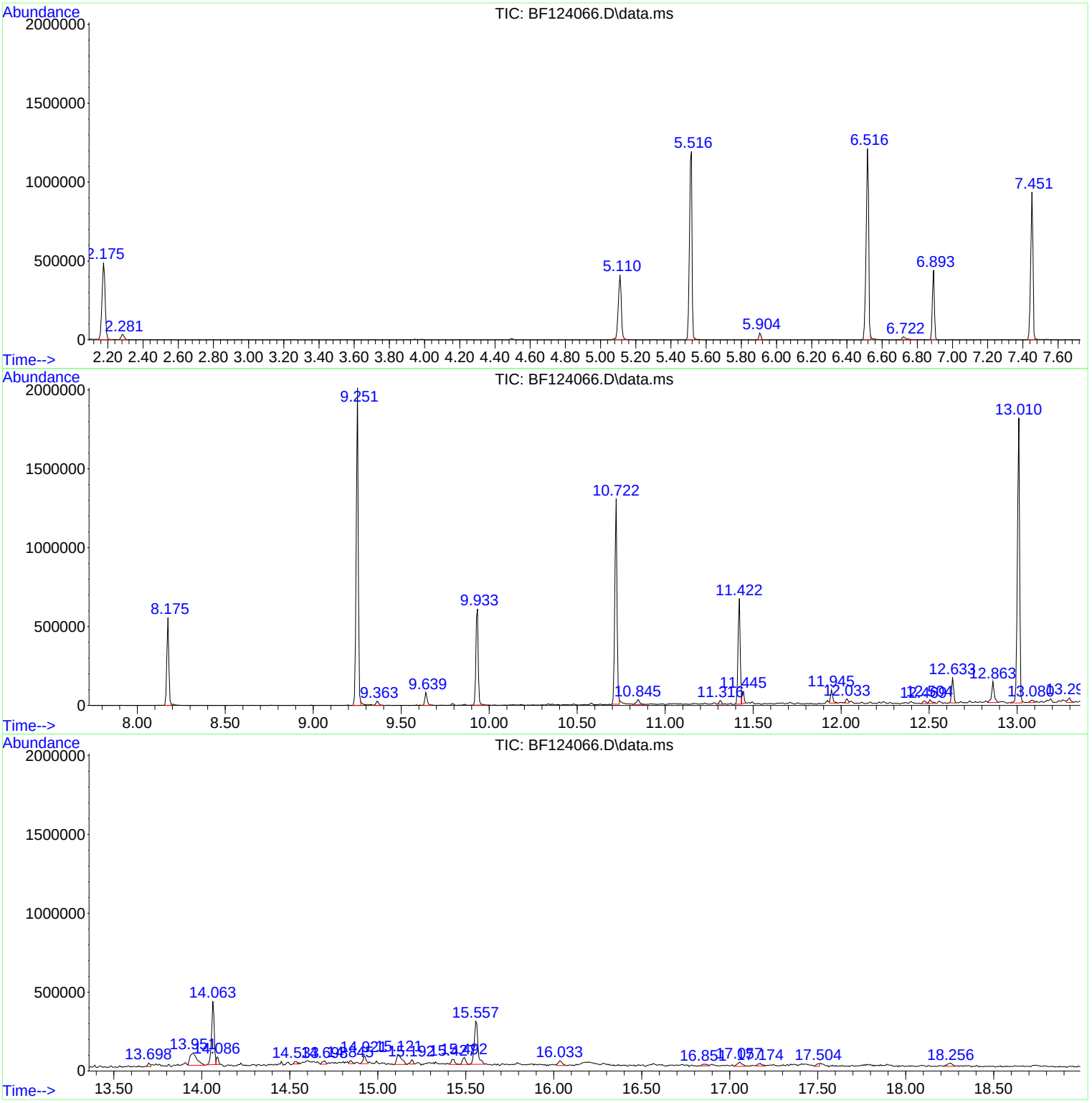
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
METRO-SP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052621\
Data File : BF124066.D
Acq On : 26 May 2021 15:43
Operator : JU/CG
Sample : M2517-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
METRO-SP

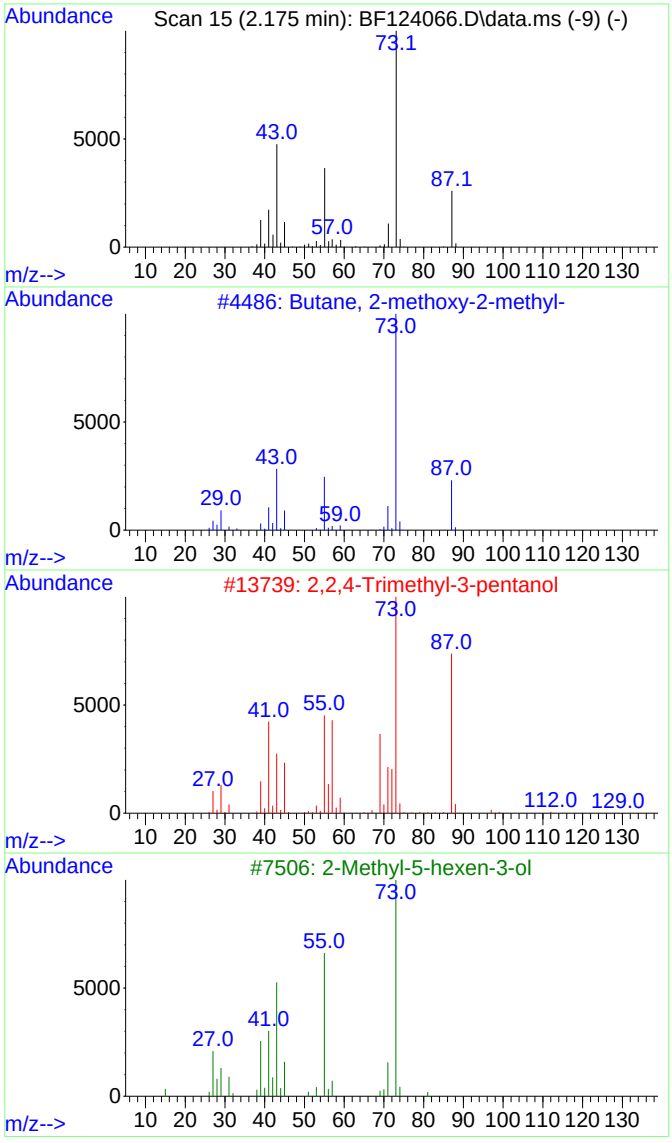
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

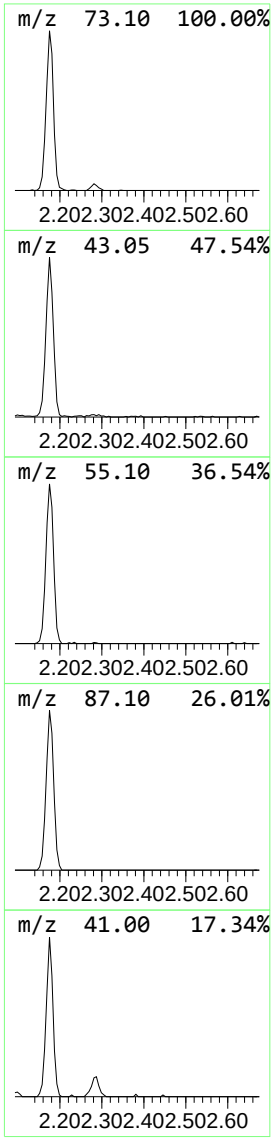
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	34.39 ng	598998	1,4-Dichlorobenzene-d4	6.893

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	40
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052621\
Data File : BF124066.D
Acq On : 26 May 2021 15:43
Operator : JU/CG
Sample : M2517-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
METRO-SP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

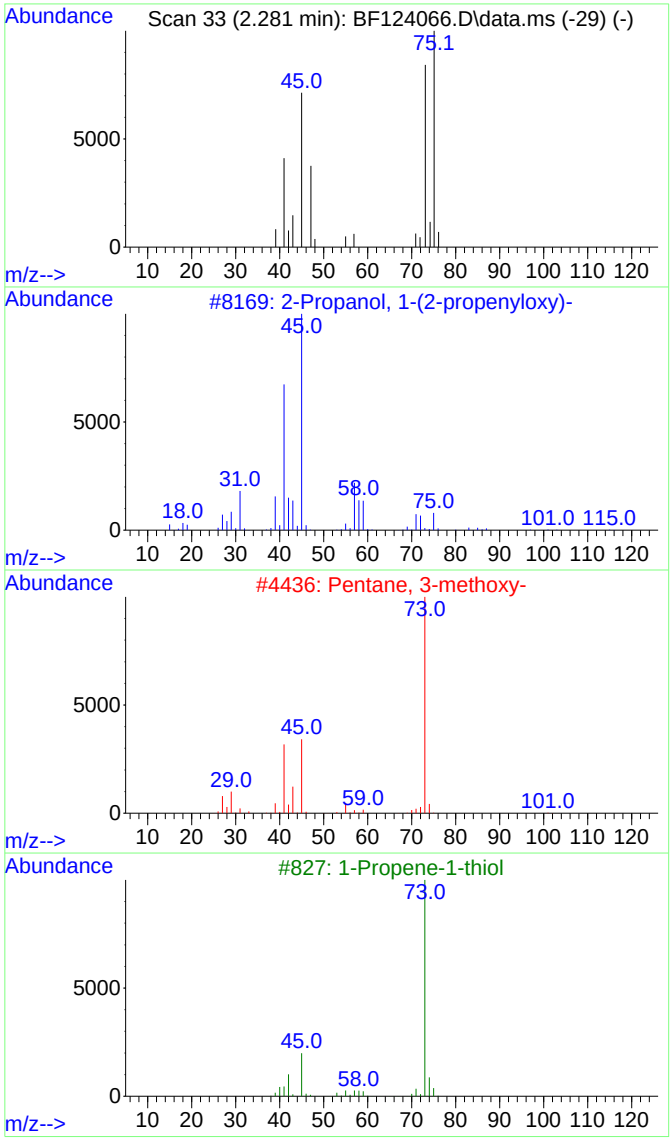
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

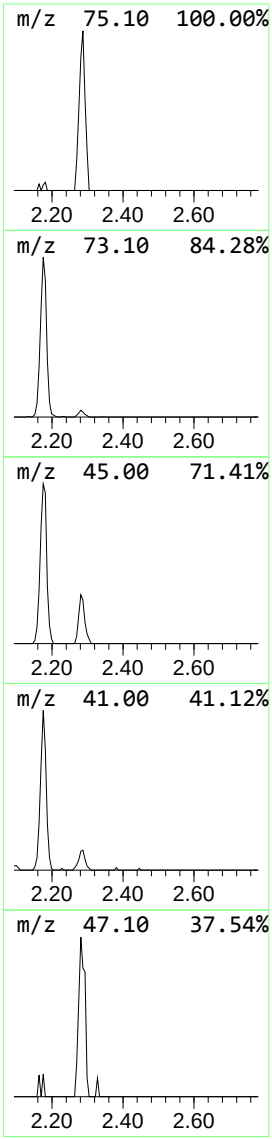
****

Peak Number 2 unknown2.28 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.281	2.43 ng	42365	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-propenyloxy)-	116	C6H12O2	021460-36-6	9
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
3	1-Propene-1-thiol	74	C3H6S	000925-89-3	5
4	Methane, nitroso-	45	CH3NO	000865-40-7	4
5	Methyl propyl ether	74	C4H10O	000557-17-5	4





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Operator : JU/CG
Sample : M2517-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : METRO-SP

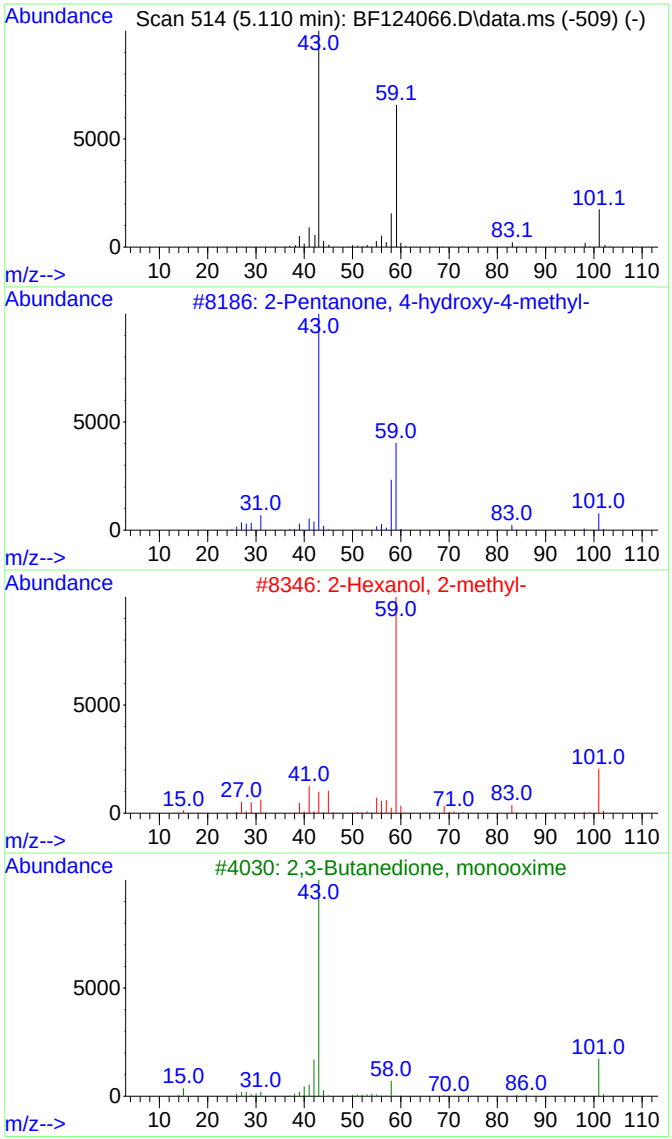
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

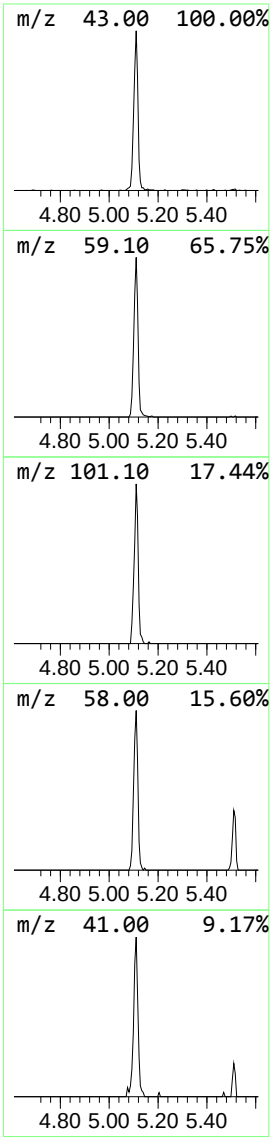
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	27.74 ng	483264	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052621\
Data File : BF124066.D
Acq On : 26 May 2021 15:43
Operator : JU/CG
Sample : M2517-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
METRO-SP

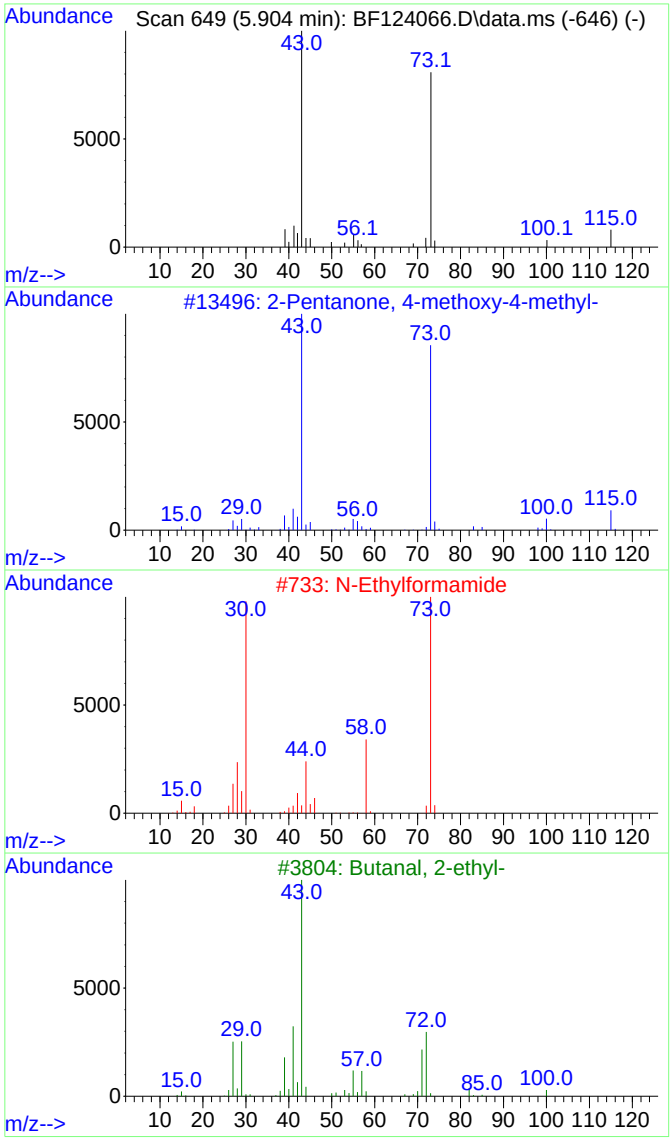
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

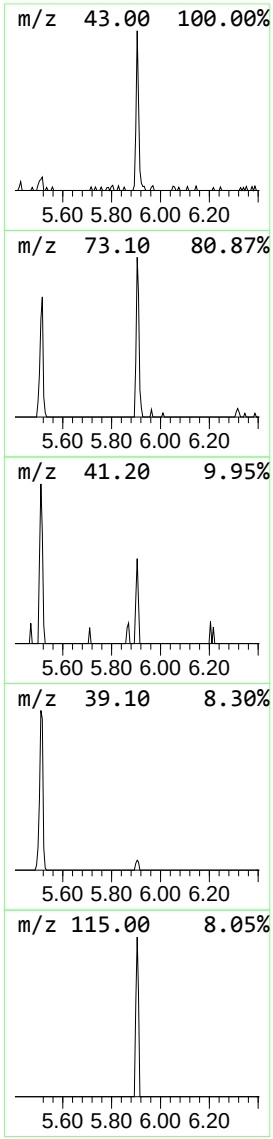
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.904	2.01 ng	35086	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2	N-Ethylformamide	73	C3H7NO	000627-45-2	23
3	Butanal, 2-ethyl-	100	C6H12O	000097-96-1	9
4	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5	Guanidine, methyl-	73	C2H7N3	000471-29-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052621\
Data File : BF124066.D
Acq On : 26 May 2021 15:43
Operator : JU/CG
Sample : M2517-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : METRO-SP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

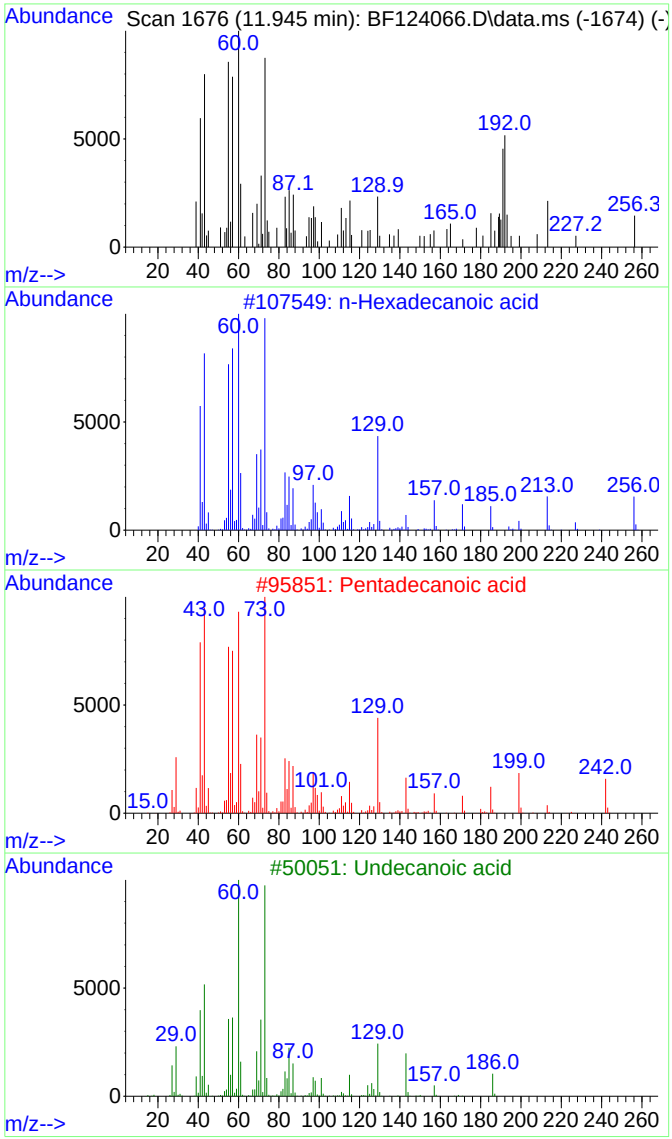
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

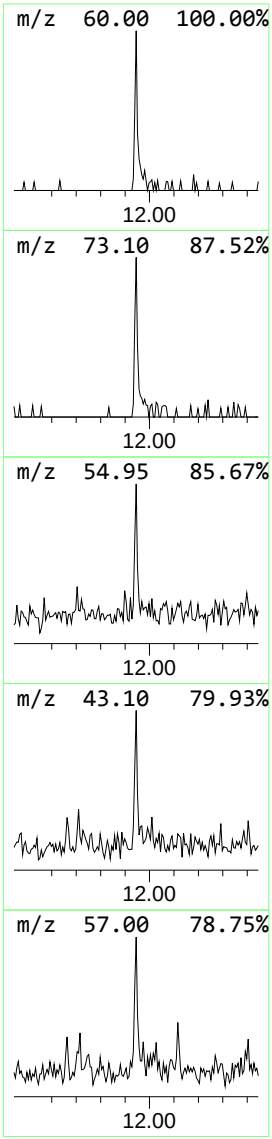
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	2.52 ng	72719	Phenanthrene-d10	11.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
3	Undecanoic acid	186	C11H22O2	000112-37-8	43
4	Dodecanoic acid	200	C12H24O2	000143-07-7	38
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	38





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Instrument : BNA_F
ClientSampleId : METRO-SP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

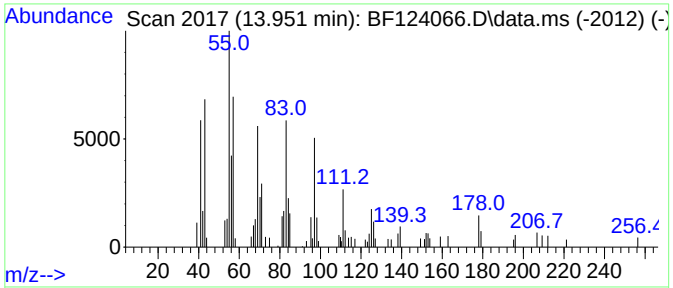
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

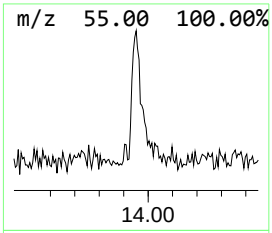
****

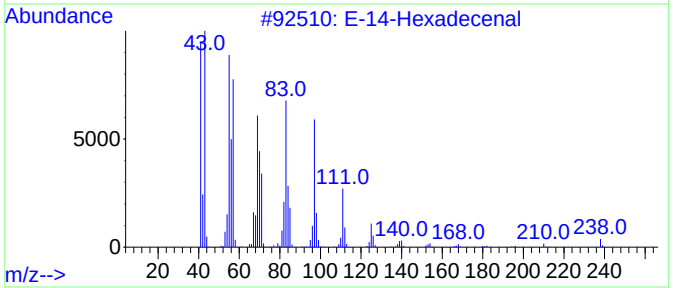
Peak Number 6 E-14-Hexadecenal Concentration Rank 3

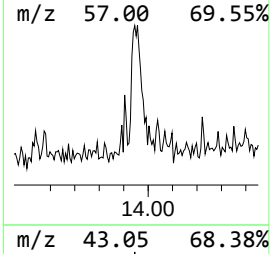
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.951	10.32 ng	216238	Chrysene-d12	14.063

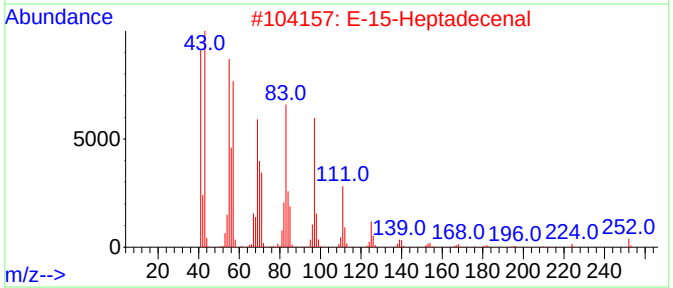
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-14-Hexadecenal	238	C16H30O	330207-53-9	72
2	E-15-Heptadecenal	252	C17H32O	1000130-97-9	72
3	1-Octadecene	252	C18H36	000112-88-9	72
4	Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	64
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	58

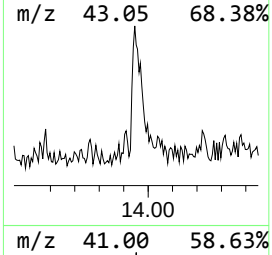


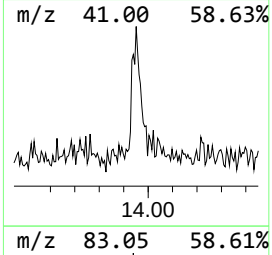


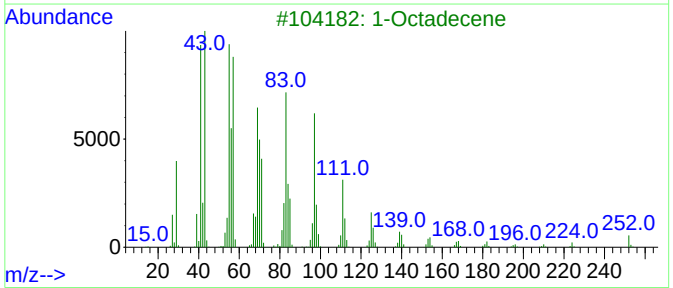


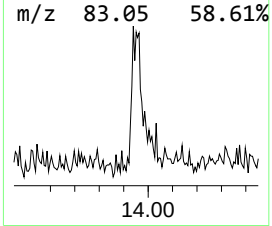












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Misc :
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

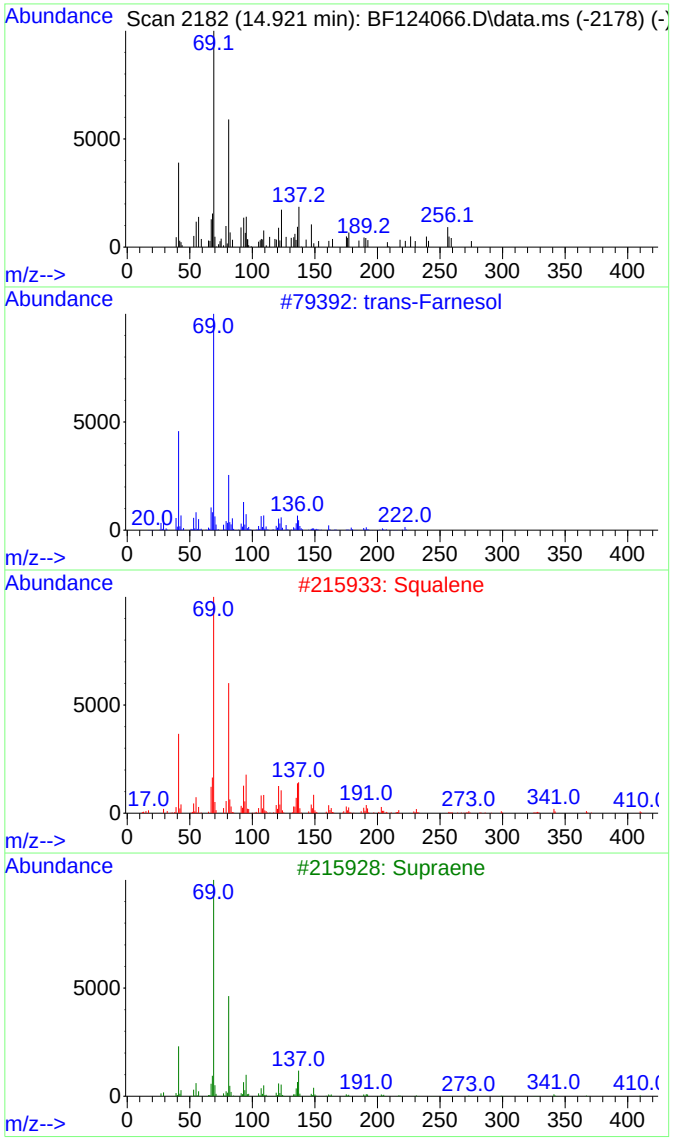
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

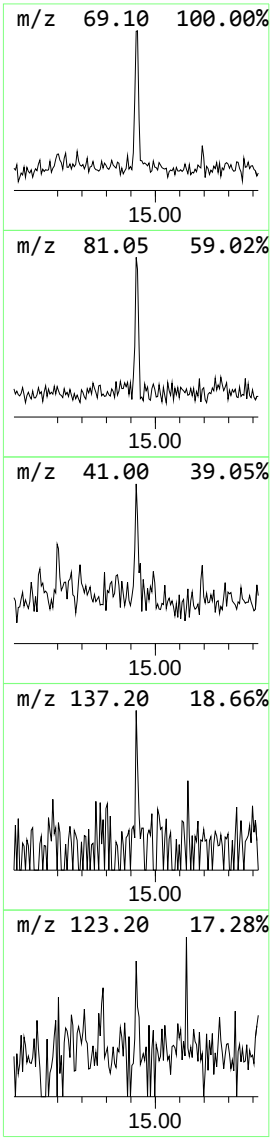
****

Peak Number 7 trans-Farnesol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.921	3.15 ng	62070	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Farnesol	222	C15H26O	000106-28-5	62
2	Squalene	410	C30H50	000111-02-4	59
3	Supraene	410	C30H50	007683-64-9	59
4	2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	47
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	45





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Data File : BF124066.D
Acq On : 26 May 2021 15:43
Operator : JU/CG
Sample : M2517-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
METRO-SP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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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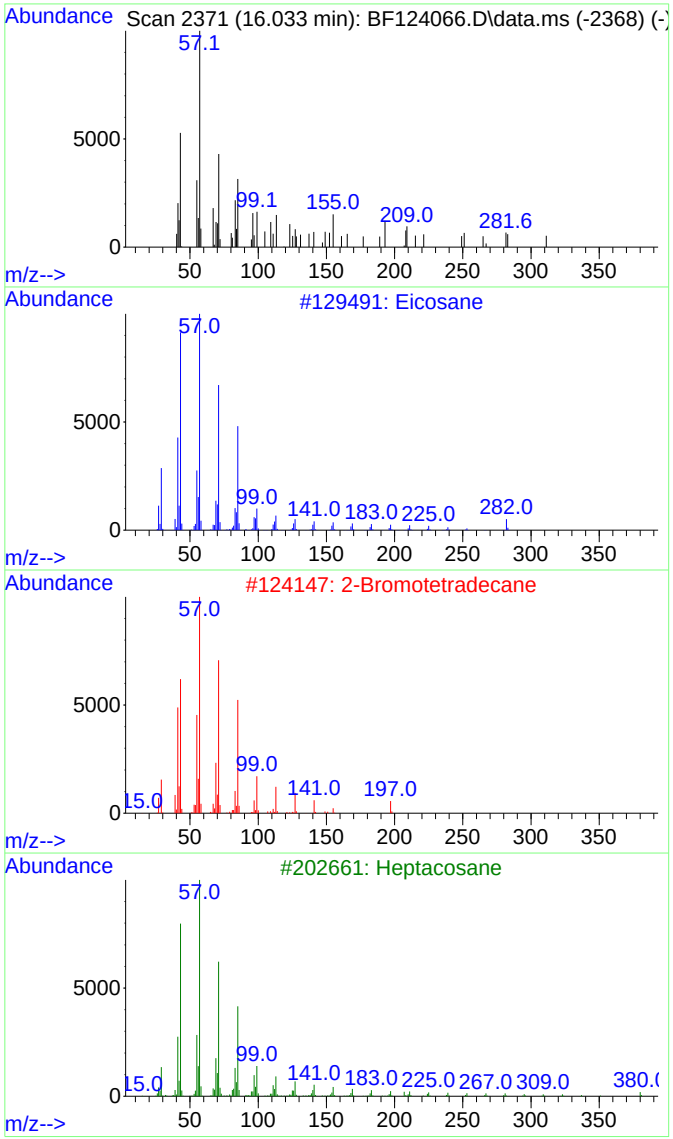
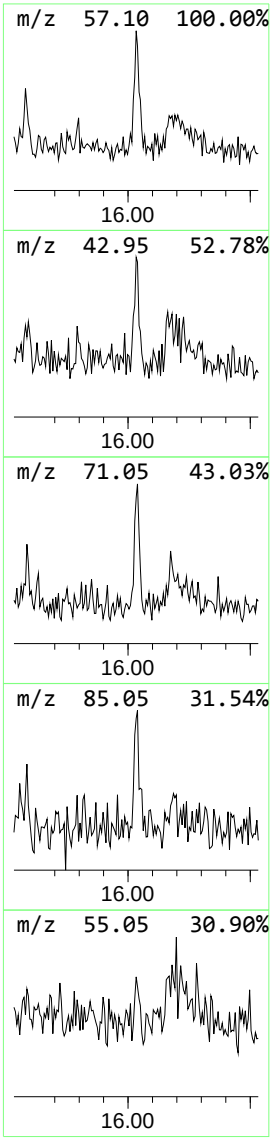
Peak Number 9 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.033	2.38 ng	47066	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	60
2	2-Bromotetradecane	276	C14H29Br	074036-95-6	46
3	Heptacosane	380	C27H56	000593-49-7	46
4	Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	43
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	43





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Data File : BF124066.D
Acq On : 26 May 2021 15:43
Operator : JU/CG
Sample : M2517-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
METRO-SP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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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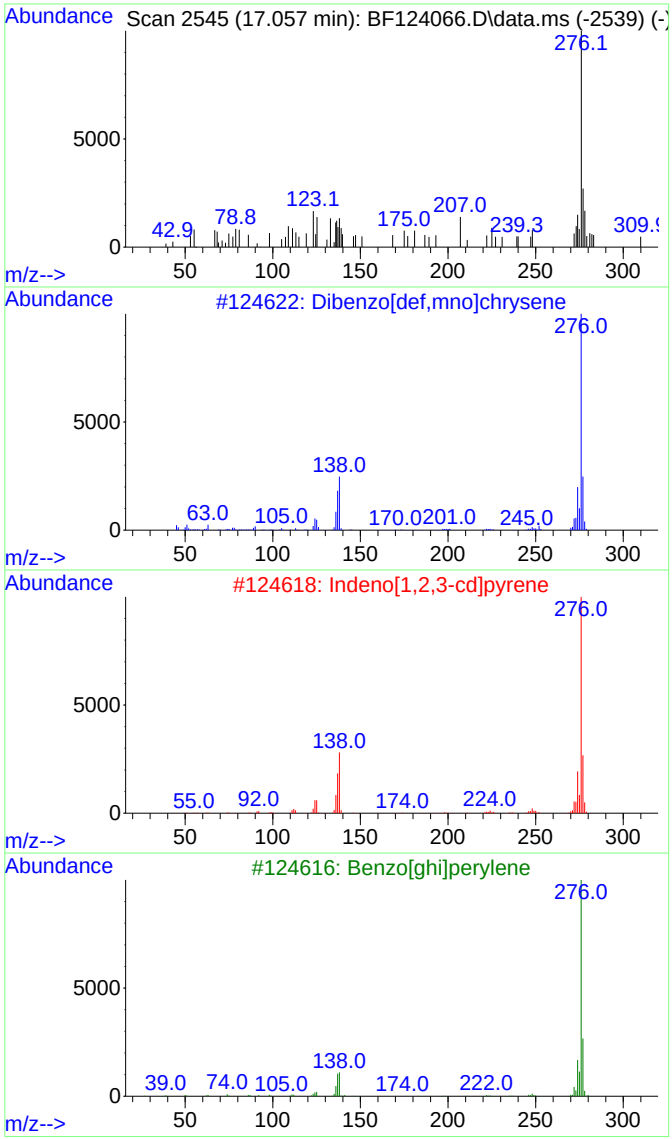
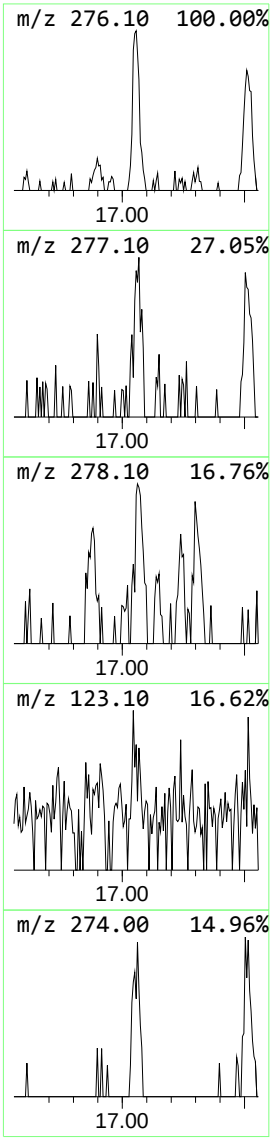
Peak Number 10 Dibenzo[def,mno]chrysene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.057	2.70 ng	53253	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	53
2	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	53
3	Benzo[ghi]perylene	276	C22H12	000191-24-2	52
4	7H-Furo[3,2-g][1]benzopyran-7-on...	276	C14H12O6	018646-72-5	47
5	Benzofuro[3,2-d]pyrimidine, 4-me...	276	C17H12N2O2	312265-36-4	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052621\
Data File : BF124066.D
Acq On : 26 May 2021 15:43
Operator : JU/CG
Sample : M2517-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : METRO-SP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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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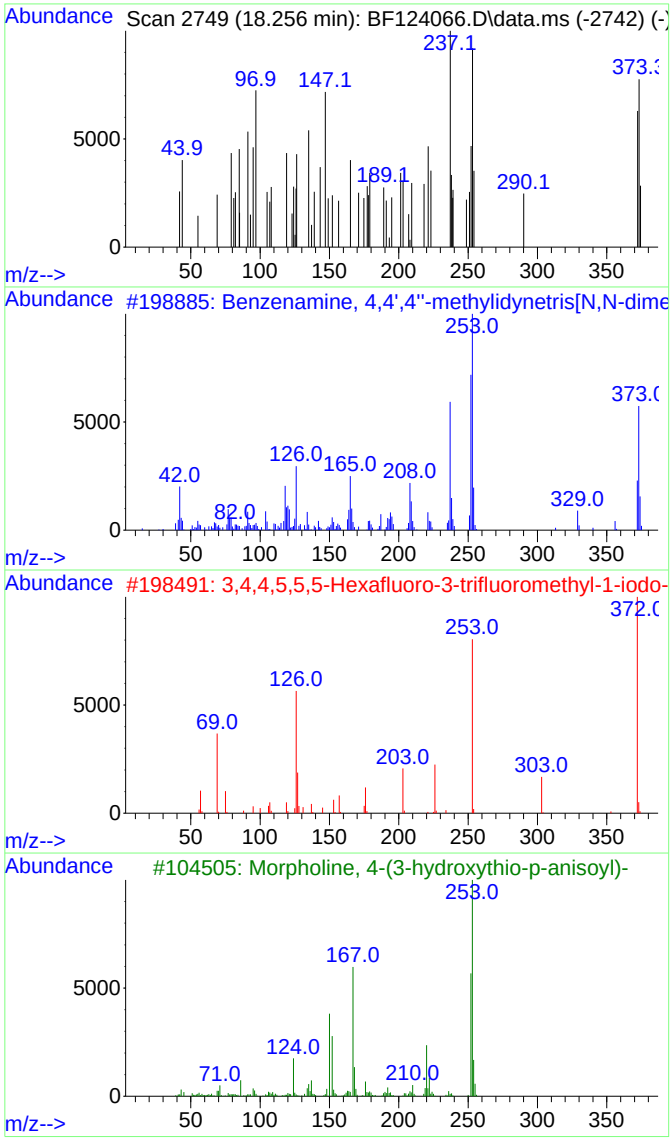
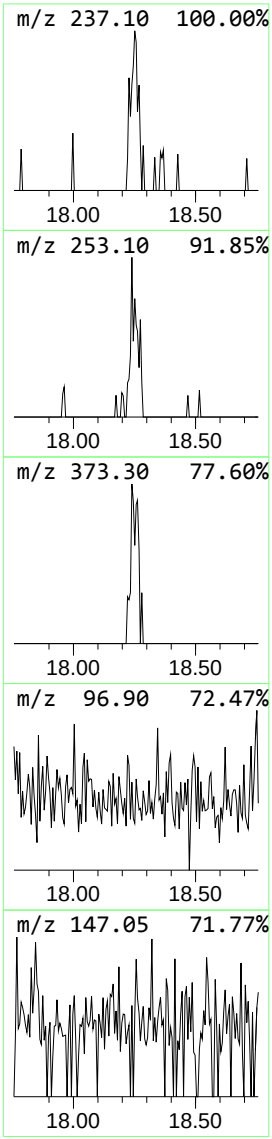
Peak Number 11 unknown18.25 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.256	2.09 ng	41310	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 4,4',4''-methylidyn...	373	C25H31N3	000603-48-5	43
2	3,4,4,5,5,5-Hexafluoro-3-trifluo...	372	C6H2F9I	239795-56-3	14
3	Morpholine, 4-(3-hydroxythio-p-a...	253	C12H15NO3S	023015-41-0	14
4	Phosphetane, 2,2,3,4,4-pentameth...	252	C14H21O2P	050517-26-5	14
5	9-Acetamido-1,8-dimethyl-3,6-dia...	237	C13H23N3O	147084-72-8	11





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052621\
Data File : BF124066.D
Acq On : 26 May 2021 15:43
Operator : JU/CG
Sample : M2517-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : METRO-SP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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
Butane, 2-metho...	2.175	34.4	ng	598998	1	6.893	348374	20.0
unknown2.28	2.281	2.4	ng	42365	1	6.893	348374	20.0
2-Pentanone, 4-...	5.110	27.7	ng	483264	1	6.893	348374	20.0
2-Pentanone, 4-...	5.904	2.0	ng	35086	1	6.893	348374	20.0
n-Hexadecanoic ...	11.945	2.5	ng	72719	4	11.422	576182	20.0
E-14-Hexadecenal	13.951	10.3	ng	216238	5	14.063	418928	20.0
trans-Farnesol	14.921	3.1	ng	62070	6	15.557	394705	20.0
Eicosane	16.033	2.4	ng	47066	6	15.557	394705	20.0
Dibenzo[def,mno...	17.057	2.7	ng	53253	6	15.557	394705	20.0
unknown18.25	18.256	2.1	ng	41310	6	15.557	394705	20.0