LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120919\
Data File : BF118148.D
Acq On : 9 Dec 2019 17:02
Operator : JU
Sample : K6162-01
Misc :
ALS Vial : 6 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-BF120619.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.075	503	508	523	rVB	287347	355229	14.28%	1.481%
2	5.481	573	577	591	rBV	1948389	1787051	71.84%	7.451%
3	6.498	745	750	769	rBV	2019280	1903826	76.54%	7.938%
4	6.634	769	773	777	rBV	2193344	2052775	82.53%	8.559%
5	6.869	809	813	816	rBV	697412	592420	23.82%	2.470%
6	7.022	835	839	843	rBV	1925929	1640976	65.97%	6.842%
7	7.428	904	908	911	rBV	1315174	1162572	46.74%	4.847%
8	8.151	1028	1031	1046	rBV	842875	769875	30.95%	3.210%
9	9.233	1211	1215	1218	rBV	2673889	2404707	96.68%	10.027%
10	9.628	1278	1282	1292	rVB	147097	133658	5.37%	0.557%
11	9.916	1327	1331	1342	rBV	1004296	922895	37.10%	3.848%
12	10.704	1461	1465	1477	rBV	1850619	1681496	67.60%	7.011%
13	11.404	1581	1584	1587	rBV	1030486	947272	38.08%	3.950%
14	11.427	1587	1588	1592	rVB	138517	92253	3.71%	0.385%
15	11.927	1667	1673	1681	rBV2	383503	429690	17.27%	1.792%
16	12.621	1788	1791	1800	rBV	201913	196349	7.89%	0.819%
17	12.716	1804	1807	1816	rBV2	157369	170820	6.87%	0.712%
18	12.851	1825	1830	1836	rVB	164237	181793	7.31%	0.758%
19	12.998	1850	1855	1858	rBV	2911314	2487411	100.00%	10.371%
20	13.698	1967	1974	1977	rBV3	21250	35605	1.43%	0.148%
21	13.892	2003	2007	2018	rVB2	261435	339106	13.63%	1.414%
22	14.057	2025	2035	2038	rBV	815052	890269	35.79%	3.712%
23	14.080	2038	2039	2050	rVB3	107461	161030	6.47%	0.671%
24	14.216	2058	2062	2068	rVB2	76649	86654	3.48%	0.361%
25	14.521	2110	2114	2120	rVB	133734	158682	6.38%	0.662%
26	14.827	2162	2166	2171	rBV	185058	200466	8.06%	0.836%
27	15.110	2210	2214	2217	rBV	54594	87335	3.51%	0.364%
28	15.174	2220	2225	2229	rBV	236051	284808	11.45%	1.188%
29	15.415	2263	2266	2271	rBV	39650	56543	2.27%	0.236%
30	15.480	2273	2277	2283	rVV	74305	113976	4.58%	0.475%
31	15.545	2283	2288	2302	rVV3	524725	1003230	40.33%	4.183%
32	16.009	2361	2367	2373	rBV	179967	286185	11.51%	1.193%
33	16.068	2374	2377	2385	rVB7	22640	41227	1.66%	0.172%
34	16.527	2450	2455	2464	rVB	91139	166714	6.70%	0.695%

LSC Area Percent Report

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Acq On : 9 Dec 2019 17:02
Operator : JU
Sample : K6162-01
Misc :
ALS Vial : 6 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-BF120619.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.051	2539	2544	2549	rBV3	24072	47927	1.93%	0.200%
36	17.133	2553	2558	2567	rVB3	38115	78210	3.14%	0.326%
37	17.504	2617	2621	2627	rVB2	18287	32265	1.30%	0.135%

Sum of corrected areas: 23983300

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120919\
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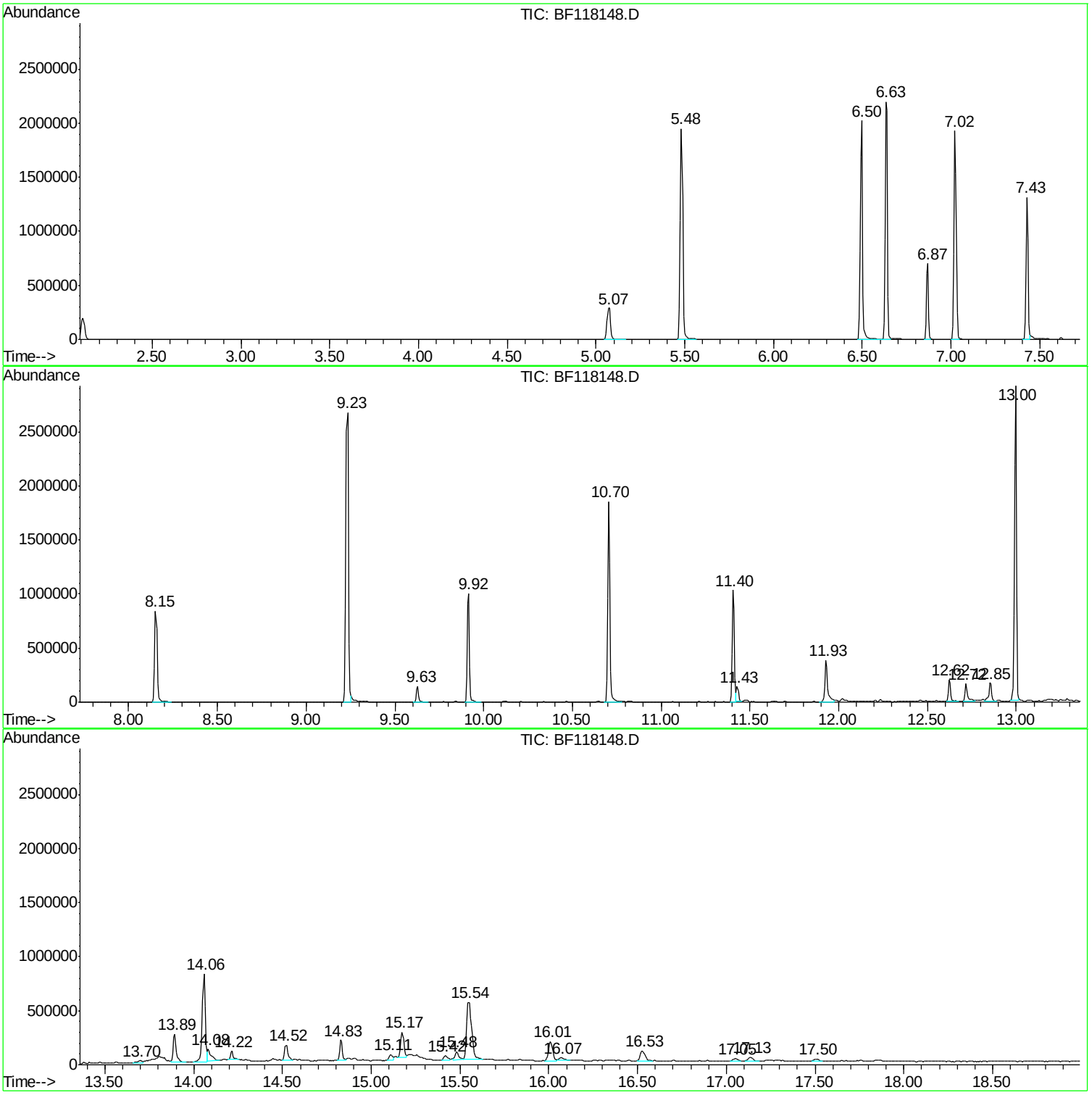
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

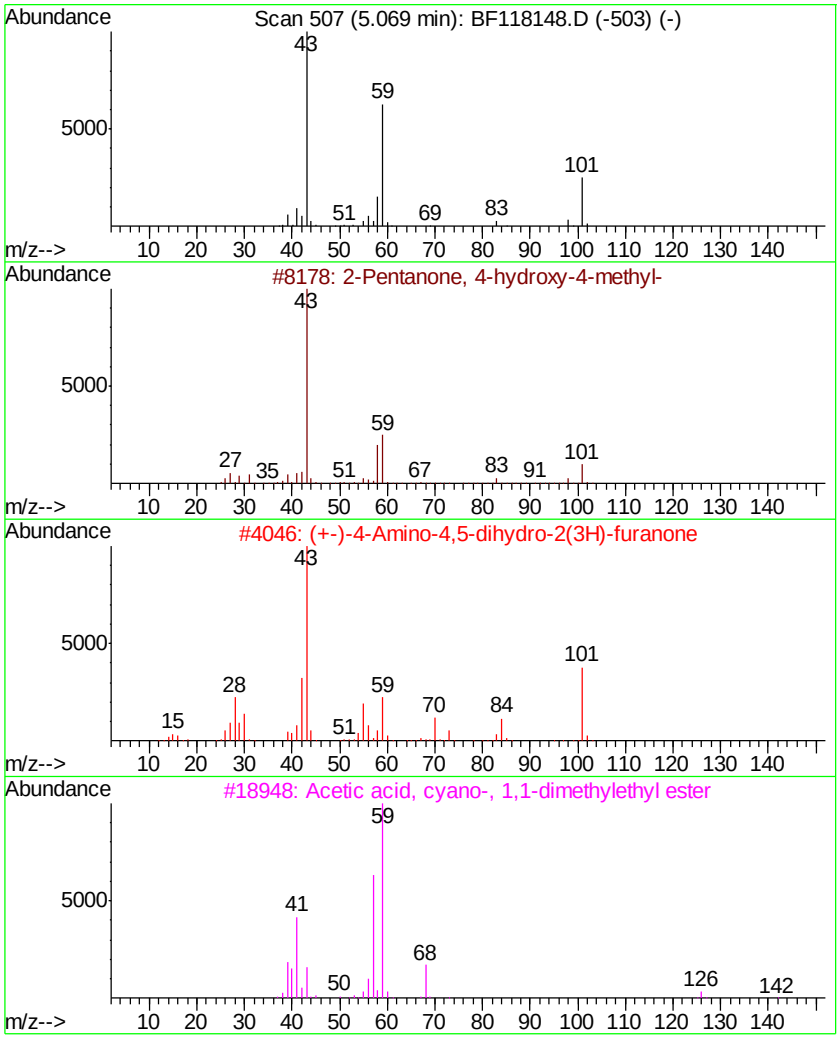
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

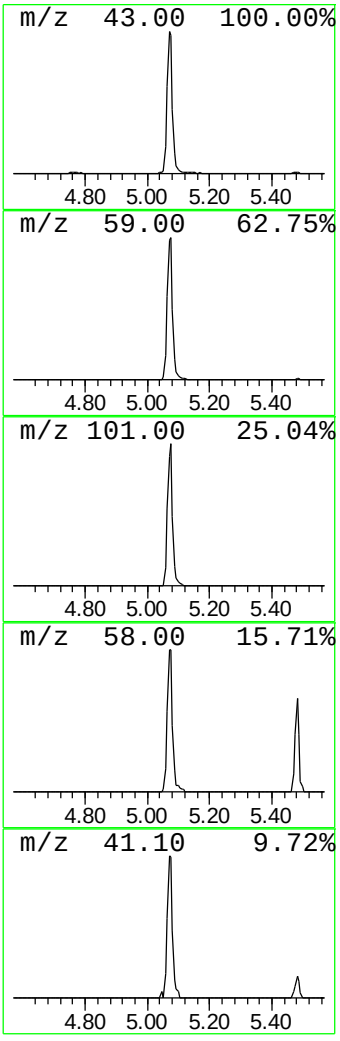
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	11.99 ng	355229	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Acetone	58	C3H6O	000067-64-1	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Acq On : 9 Dec 2019 17:02
Operator : JU
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

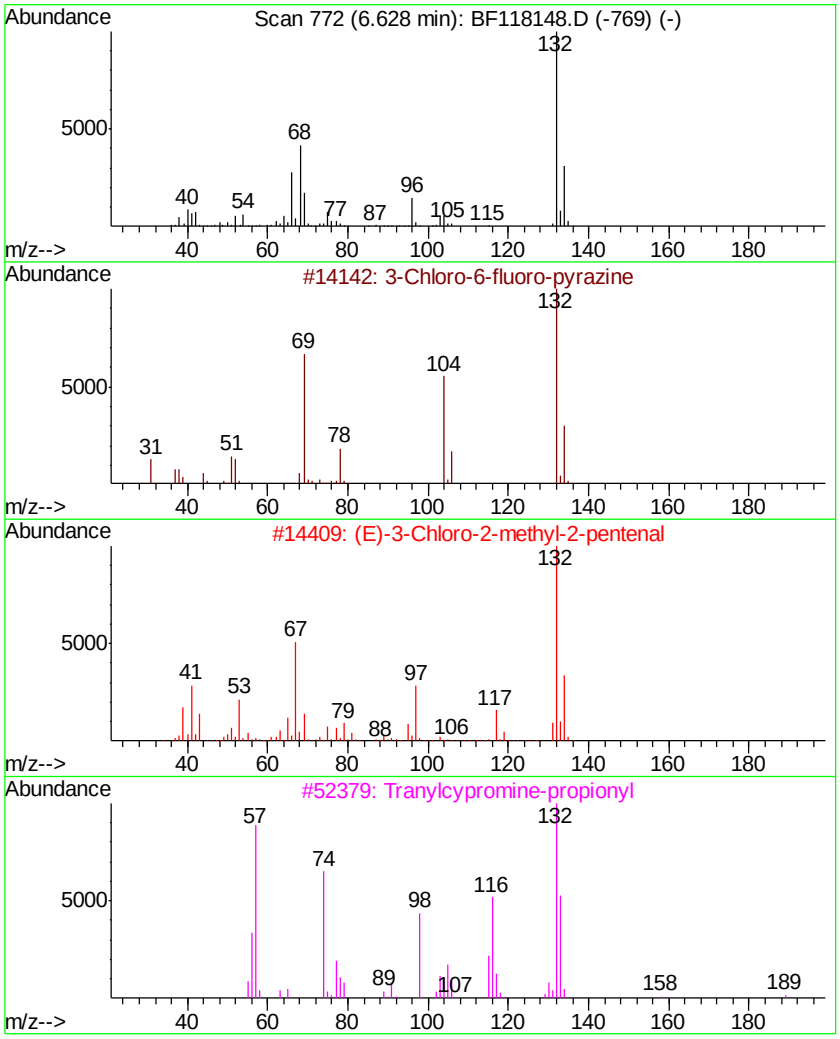
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

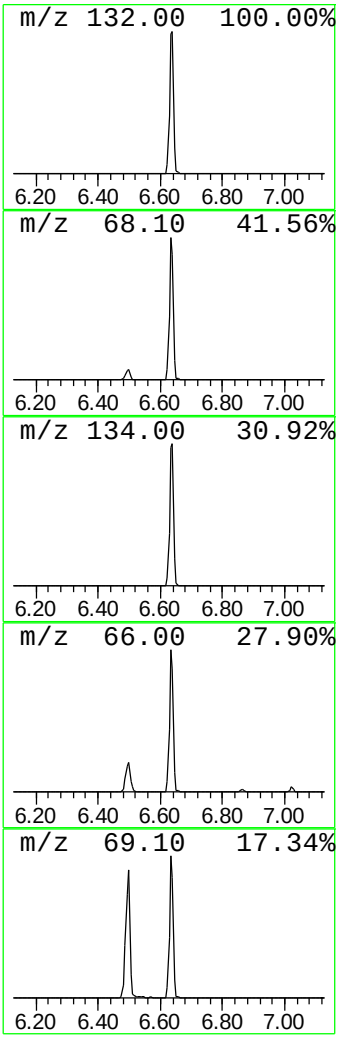
****

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	69.30 ng	2052780	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120919\
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Operator : JU
Sample : K6162-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

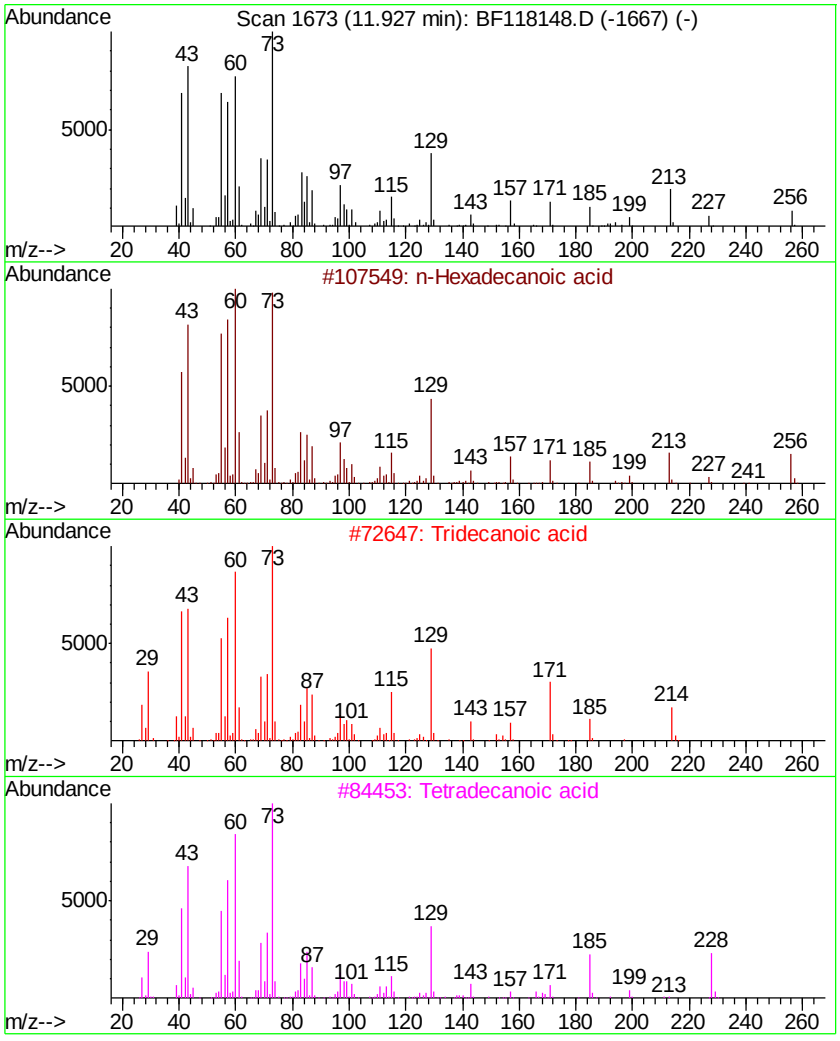
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

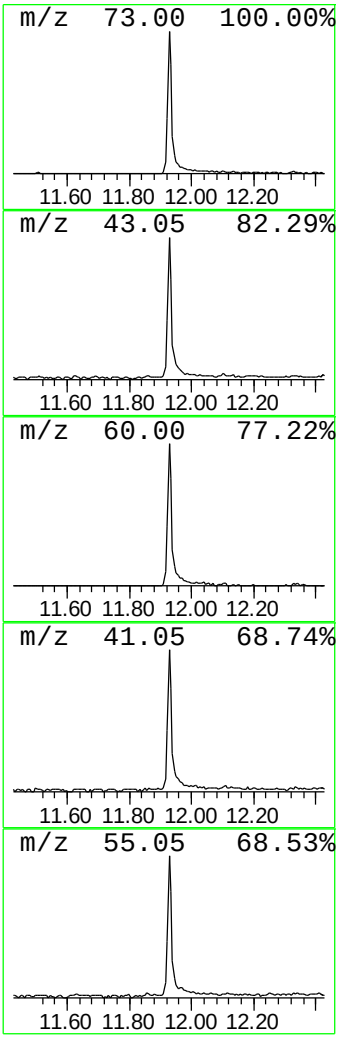
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	9.07 ng	429690	Phenanthrene-d10	11.40

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	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	60
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	59





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Operator : JU
Sample : K6162-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

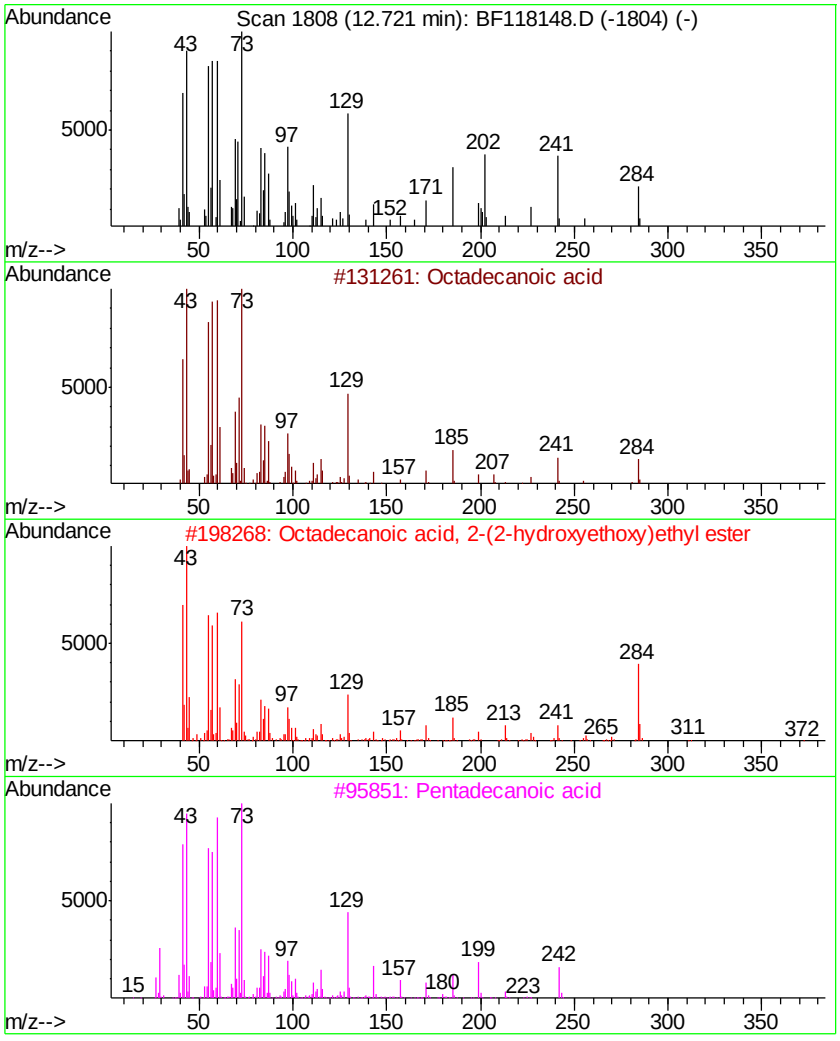
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

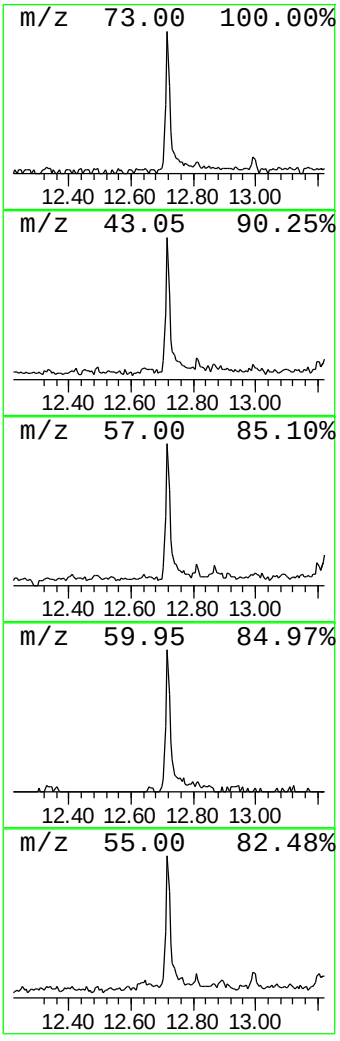
****

Peak Number 5 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	3.61 ng	170820	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





Library Search Compound Report

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ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

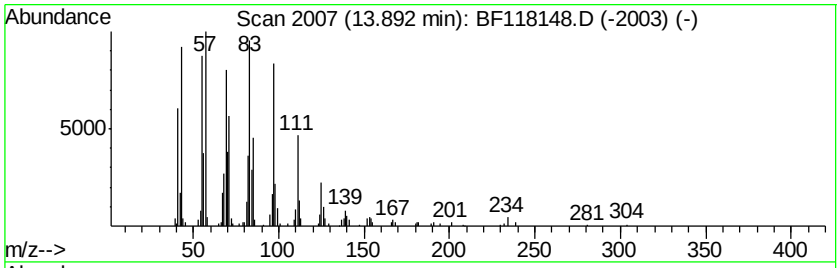
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

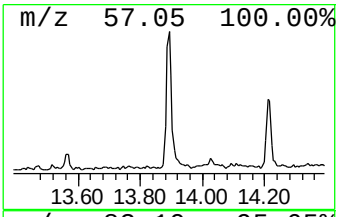
****

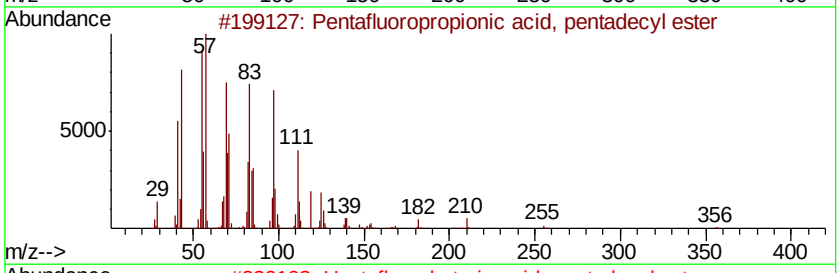
Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 5

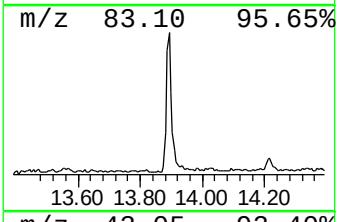
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	7.62 ng	339106	Chrysene-d12	14.06

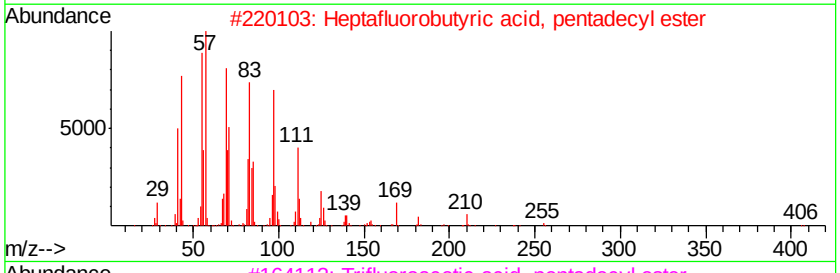
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	93

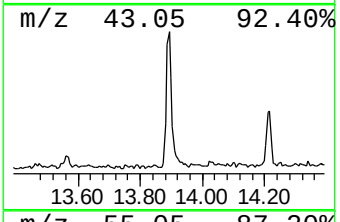


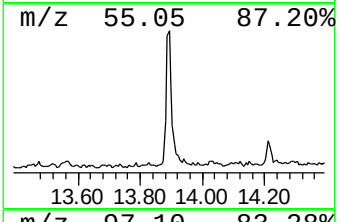


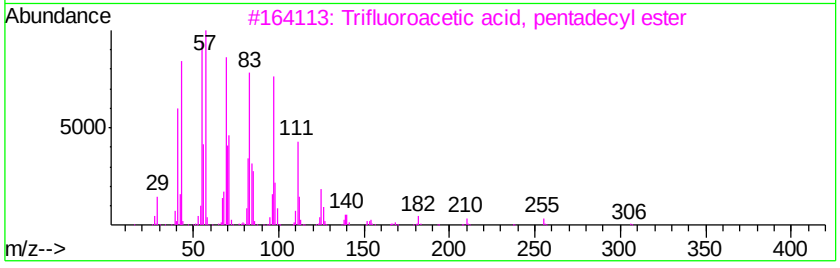


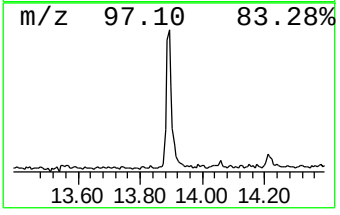












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

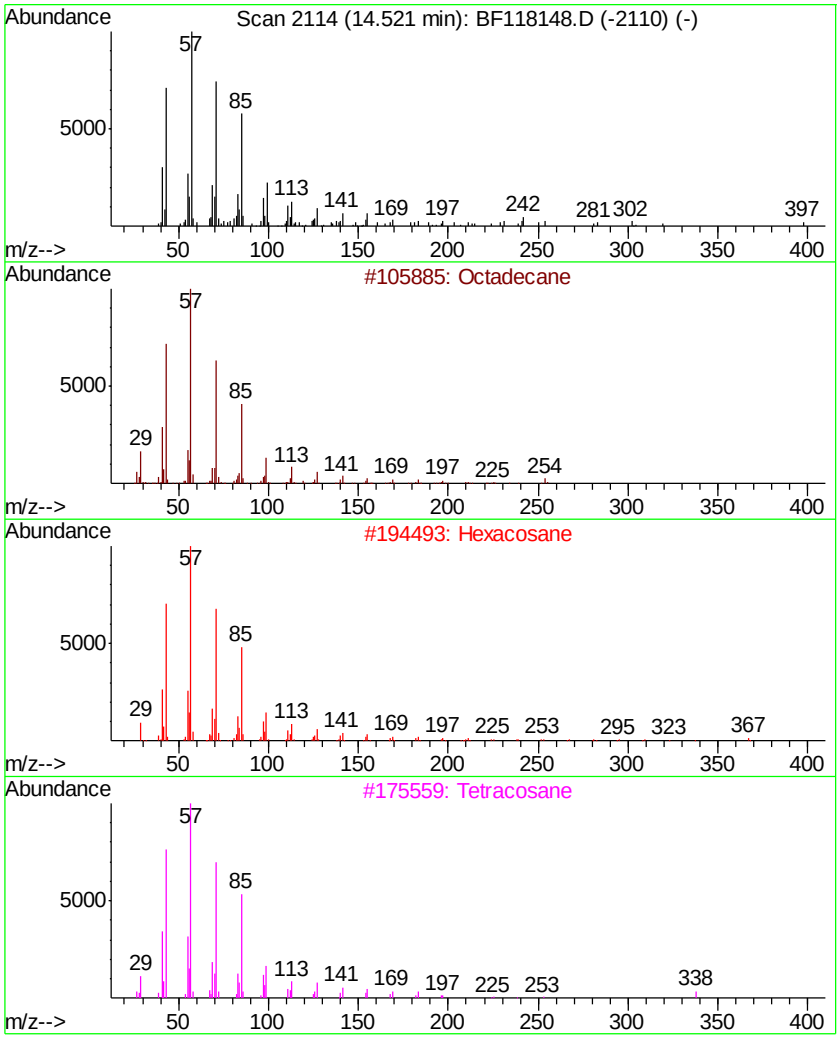
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

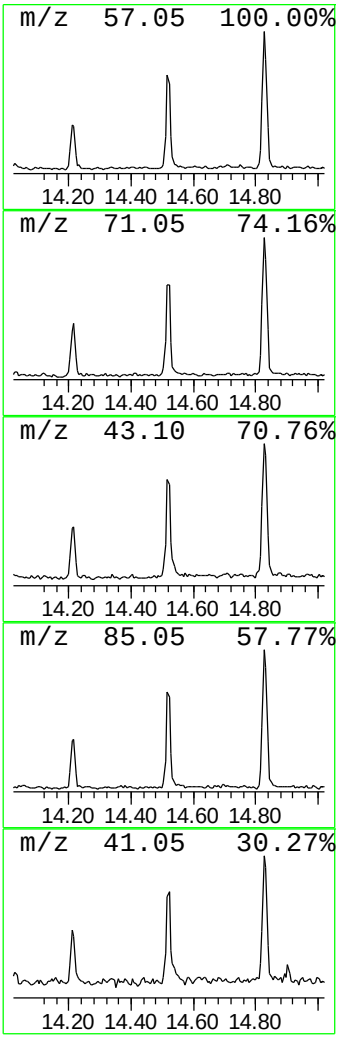
****

Peak Number 7 Octadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	3.56 ng	158682	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	96
2	Hexacosane	366	C26H54	000630-01-3	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Octacosane	394	C28H58	000630-02-4	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





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Instrument : BNA_F
ClientSampleId : TP1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

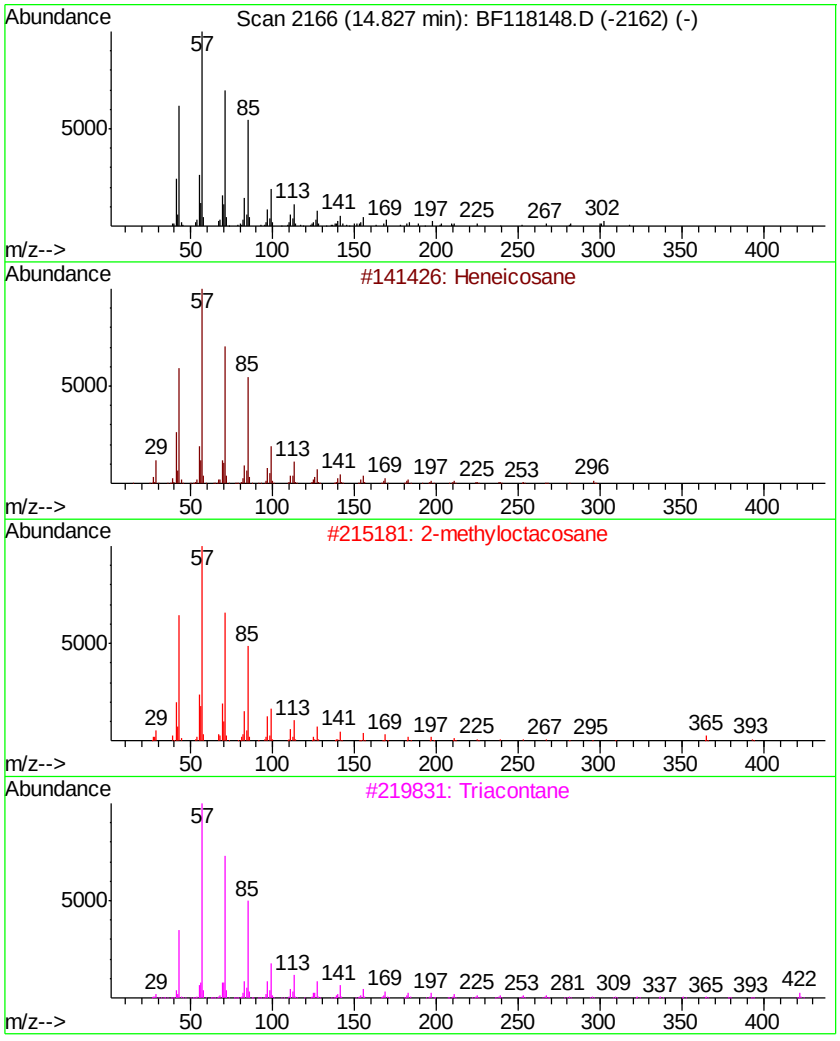
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

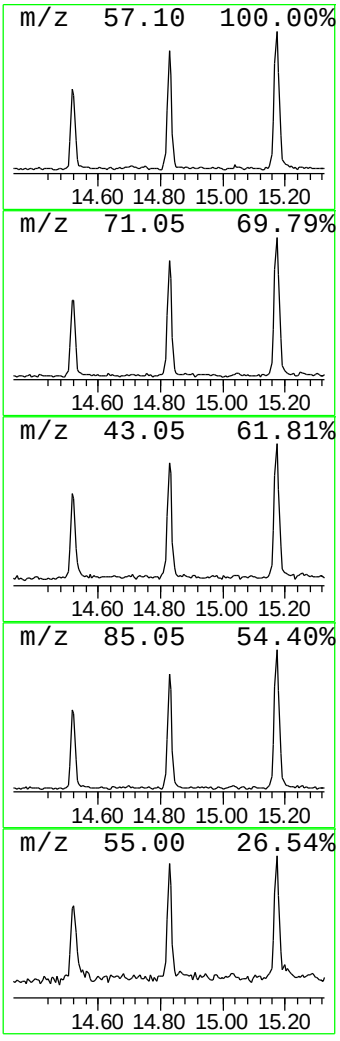
****

Peak Number 8 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	4.00 ng	200466	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	2-methyloctacosane	408	C29H60	1000376-72-8	87
3	Triacontane	422	C30H62	000638-68-6	87
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5	Hexacosane	366	C26H54	000630-01-3	87





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ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP1

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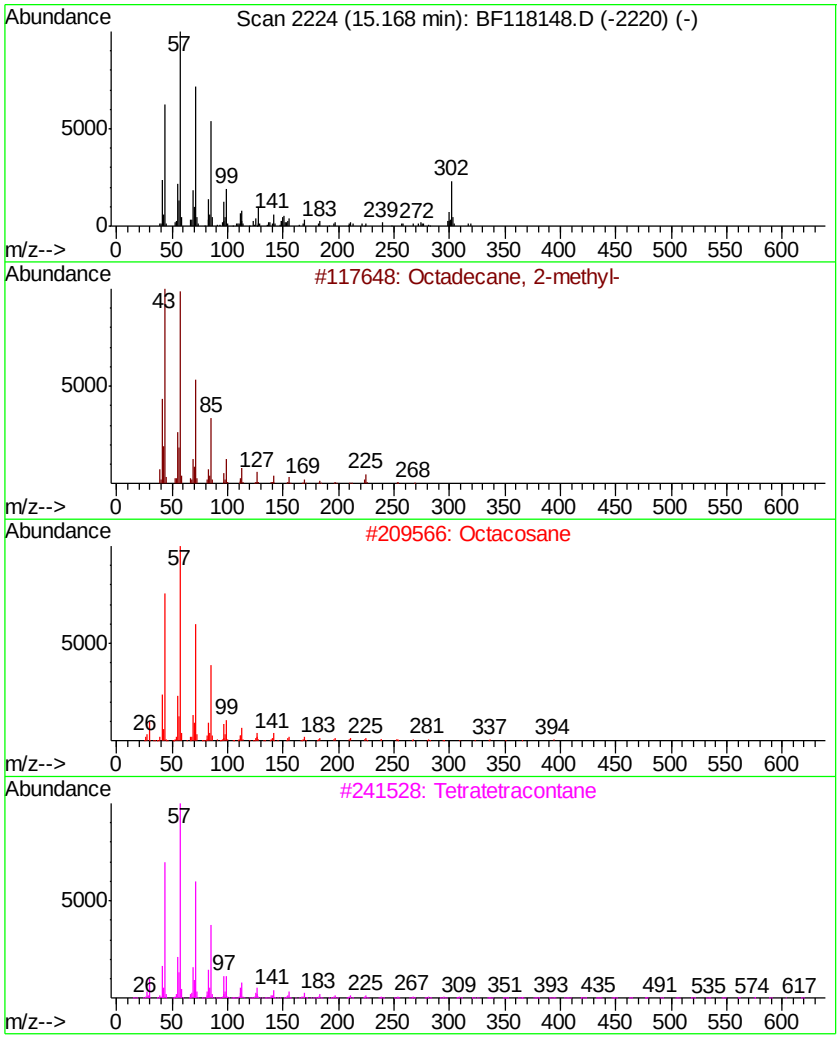
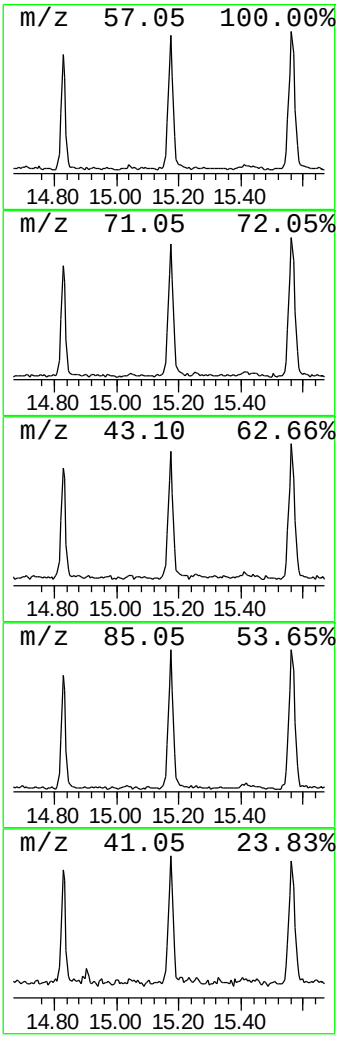
Peak Number 9 Octadecane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	5.68 ng	284808	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2-methyl-	268	C19H40	001560-88-9	83
2	Octacosane	394	C28H58	000630-02-4	81
3	Tetratetracontane	619	C44H90	007098-22-8	81
4	Hexacosane	366	C26H54	000630-01-3	81
5	Heptacosane	380	C27H56	000593-49-7	81





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120919\
Data File : BF118148.D
Acq On : 9 Dec 2019 17:02
Operator : JU
Sample : K6162-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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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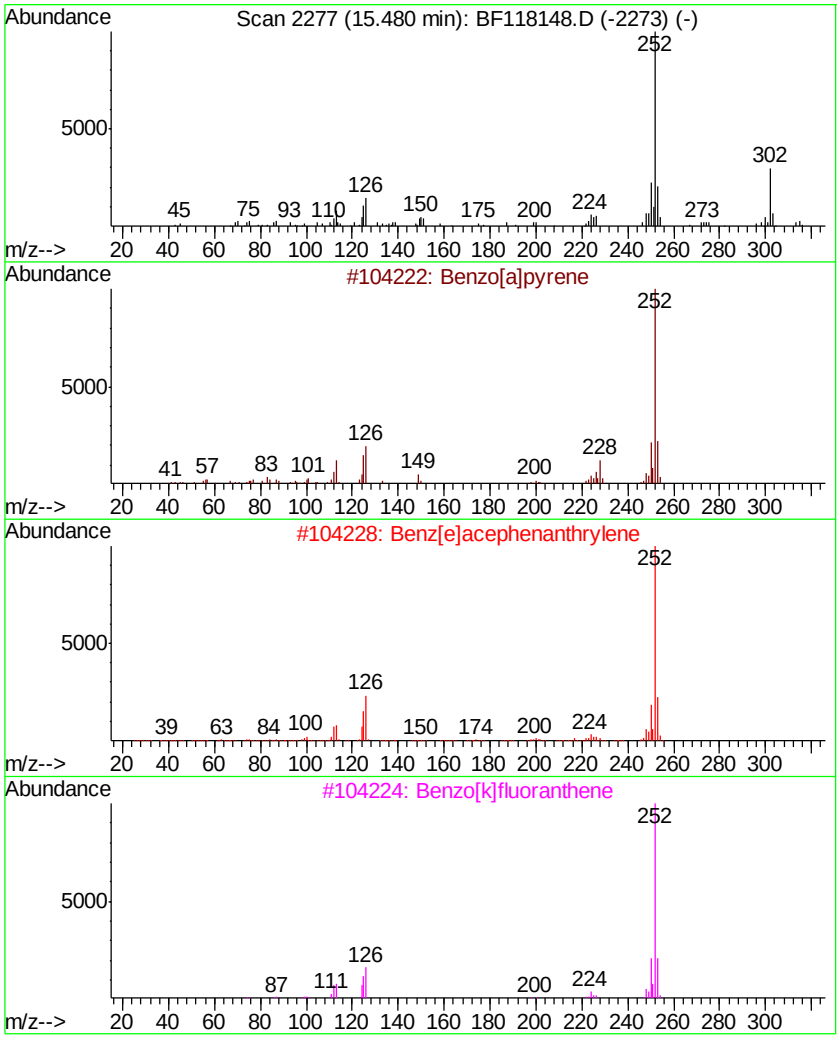
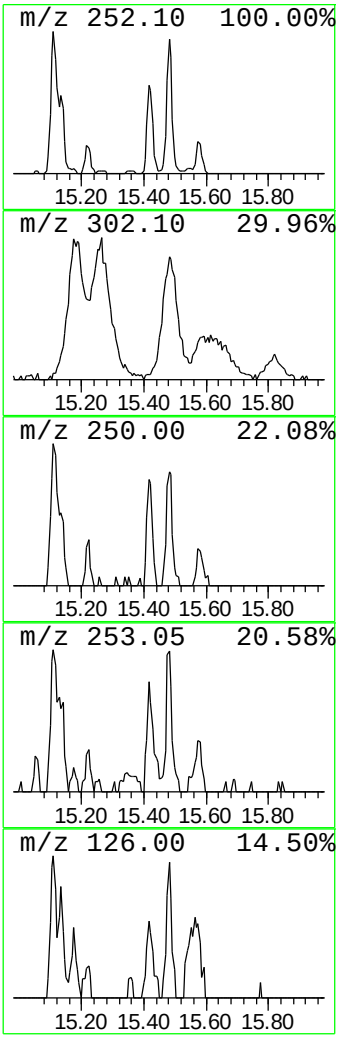
Peak Number 10 Benzo[e]pyrene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.48	2.27 ng	113976	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene	252	C20H12	000050-32-8	93
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	91
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	83
4	(1-Cyclopentenyl)ferrocene	252	C15H16Fe	012260-67-2	72
5	Benzo[e]pyrene	252	C20H12	000192-97-2	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120919\
Data File : BF118148.D
Acq On : 9 Dec 2019 17:02
Operator : JU
Sample : K6162-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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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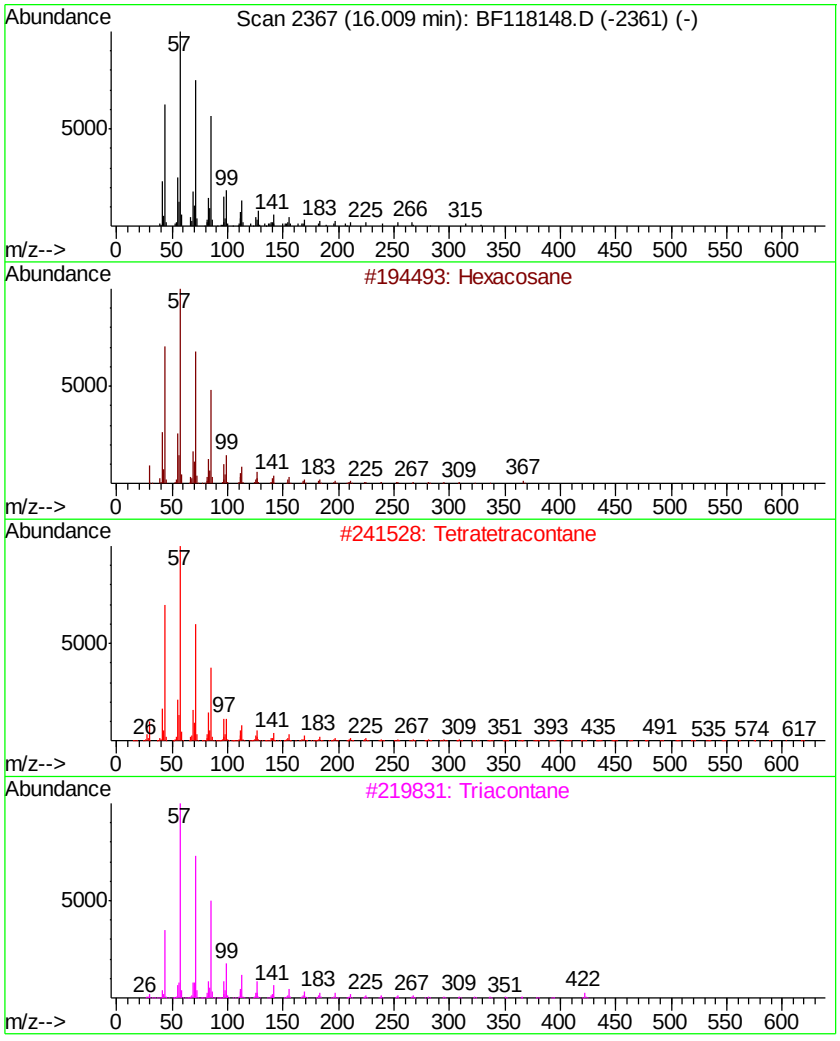
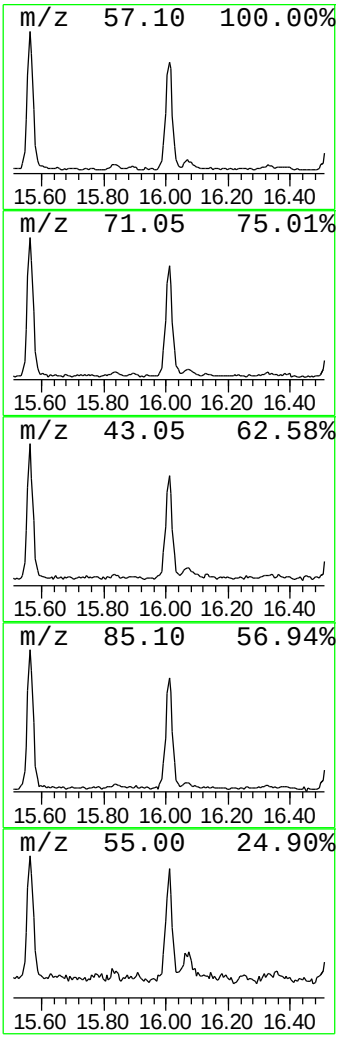
Peak Number 11 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.01	5.71 ng	286185	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	94
2	Tetratetracontane	619	C44H90	007098-22-8	91
3	Triacontane	422	C30H62	000638-68-6	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Eicosane	282	C20H42	000112-95-8	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120919\
Data File : BF118148.D
Acq On : 9 Dec 2019 17:02
Operator : JU
Sample : K6162-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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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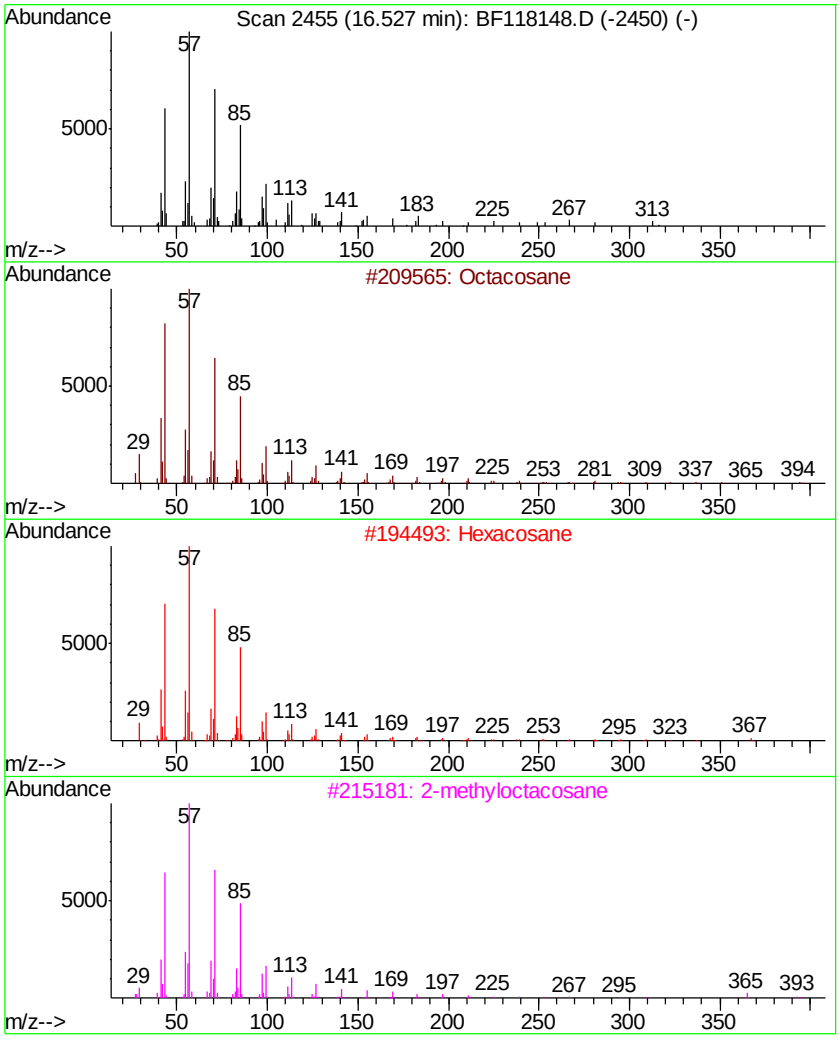
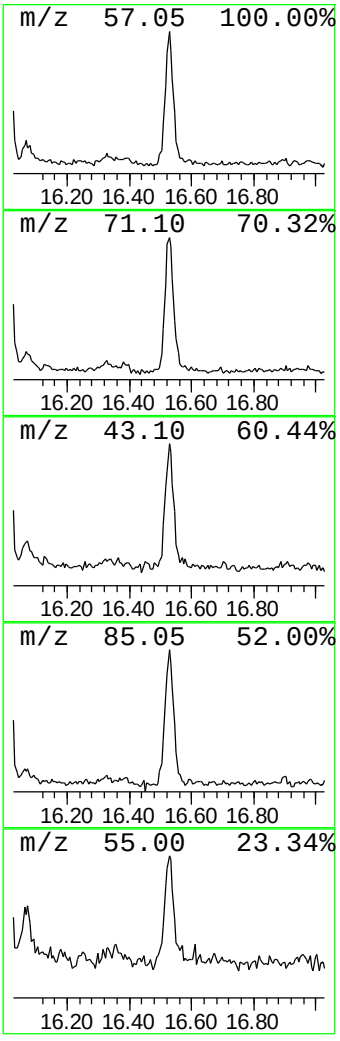
Peak Number 12 2-methyloctacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	3.32 ng	166714	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hexacosane	366	C26H54	000630-01-3	90
3	2-methyloctacosane	408	C29H60	1000376-72-8	87
4	Triacontane	422	C30H62	000638-68-6	87
5	Heneicosane	296	C21H44	000629-94-7	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF120919\
Data File : BF118148.D
Acq On : 9 Dec 2019 17:02
Operator : JU
Sample : K6162-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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
2-Pentanone, 4-hy...	5.07	12.0	ng	355229	1	6.87	592420	20.0
unknown6.63	6.63	69.3	ng	2052780	1	6.87	592420	20.0
n-Hexadecanoic acid	11.93	9.1	ng	429690	4	11.40	947272	20.0
Octadecanoic acid	12.72	3.6	ng	170820	4	11.40	947272	20.0
Pentafluoropropio...	13.89	7.6	ng	339106	5	14.06	890269	20.0
Octadecane	14.52	3.6	ng	158682	5	14.06	890269	20.0
Heneicosane	14.83	4.0	ng	200466	6	15.54	1003230	20.0
Octadecane, 2-met...	15.17	5.7	ng	284808	6	15.54	1003230	20.0
Benzo[e]pyrene	15.48	2.3	ng	113976	6	15.54	1003230	20.0
Hexacosane	16.01	5.7	ng	286185	6	15.54	1003230	20.0
2-methyloctacosane	16.53	3.3	ng	166714	6	15.54	1003230	20.0