LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110518\
Data File : BF110471.D
Acq On : 5 Nov 2018 18:03
Operator : JU/SJ
Sample : J5812-25
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP4-A

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-BF102318.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	2.316	31	39	48	rBV	419122	562369	18.87%	2.131%
2	5.204	527	530	540	rBV	73716	107516	3.61%	0.408%
3	5.581	590	594	598	rBV	2326503	2409413	80.86%	9.132%
4	6.581	758	764	779	rBV	2256173	2771809	93.03%	10.506%
5	6.728	784	789	792	rBV	2719156	2635637	88.46%	9.989%
6	6.951	824	827	832	rBV	663819	554688	18.62%	2.102%
7	7.110	849	854	857	rBV	2268780	1994915	66.95%	7.561%
8	7.522	918	924	943	rBV	1459555	1721376	57.77%	6.524%
9	8.239	1041	1046	1065	rVB	643044	758093	25.44%	2.873%
10	9.239	1210	1216	1222	rBV	33370	39804	1.34%	0.151%
11	9.310	1222	1228	1231	rBV	3288470	2979626	100.00%	11.293%
12	9.375	1237	1239	1242	rVB2	33898	32105	1.08%	0.122%
13	9.622	1277	1281	1284	rBV	90480	85533	2.87%	0.324%
14	9.698	1289	1294	1300	rBV	338583	386684	12.98%	1.466%
15	9.851	1314	1320	1322	rBV3	21329	31717	1.06%	0.120%
16	9.898	1322	1328	1331	rVV4	37733	58275	1.96%	0.221%
17	9.992	1338	1344	1348	rBV	868339	874820	29.36%	3.316%
18	10.027	1348	1350	1357	rVB	45453	52338	1.76%	0.198%
19	10.545	1436	1438	1445	rVB	34125	31964	1.07%	0.121%
20	10.622	1447	1451	1454	rBV	42953	47991	1.61%	0.182%
21	10.792	1475	1480	1492	rBV	1859161	1911831	64.16%	7.246%
22	10.886	1492	1496	1500	rVV	68742	84759	2.84%	0.321%
23	11.486	1594	1598	1601	rBV	917620	854969	28.69%	3.240%
24	11.510	1601	1602	1606	rVV	166982	115946	3.89%	0.439%
25	11.563	1610	1611	1616	rVB	48763	51763	1.74%	0.196%
26	11.992	1681	1684	1686	rBV3	57626	60046	2.02%	0.228%
27	12.104	1700	1703	1706	rBV	48189	48229	1.62%	0.183%
28	12.633	1790	1793	1796	rBV	44500	44143	1.48%	0.167%
29	12.704	1801	1805	1808	rBV	313852	273750	9.19%	1.038%
30	12.933	1838	1844	1850	rVB	234526	267912	8.99%	1.015%
31	13.068	1862	1867	1870	rBV	2623058	2487525	83.48%	9.428%
32	13.263	1893	1900	1906	rVV2	41102	81248	2.73%	0.308%
33	13.327	1908	1911	1914	rBV	37535	32215	1.08%	0.122%
34	13.380	1914	1920	1925	rVB5	17146	42877	1.44%	0.163%

LSC Area Percent Report

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Sample : J5812-25
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP4-A

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-BF102318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.492	1936	1939	1943	rBV	121451	119131	4.00%	0.452%
36	13.945	2013	2016	2025	rBV3	141593	201333	6.76%	0.763%
37	14.133	2043	2048	2051	rBV	598709	603661	20.26%	2.288%
38	14.562	2117	2121	2123	rBV2	42382	44450	1.49%	0.168%
39	14.880	2172	2175	2179	rVB	39304	36797	1.23%	0.139%
40	15.204	2226	2230	2232	rBV	35981	51065	1.71%	0.194%
41	15.227	2232	2234	2240	rVB	75257	88478	2.97%	0.335%
42	15.592	2292	2296	2298	rBV2	25120	34539	1.16%	0.131%
43	15.627	2298	2302	2303	rVV	49675	60955	2.05%	0.231%
44	15.656	2303	2307	2319	rVB2	306851	449421	15.08%	1.703%
45	16.080	2373	2379	2387	rVB	55228	85972	2.89%	0.326%
46	16.609	2464	2469	2478	rVB3	29422	50540	1.70%	0.192%
47	17.233	2569	2575	2583	rVB8	25487	63948	2.15%	0.242%

Sum of corrected areas: 26384176

LSC Report - Integrated Chromatogram

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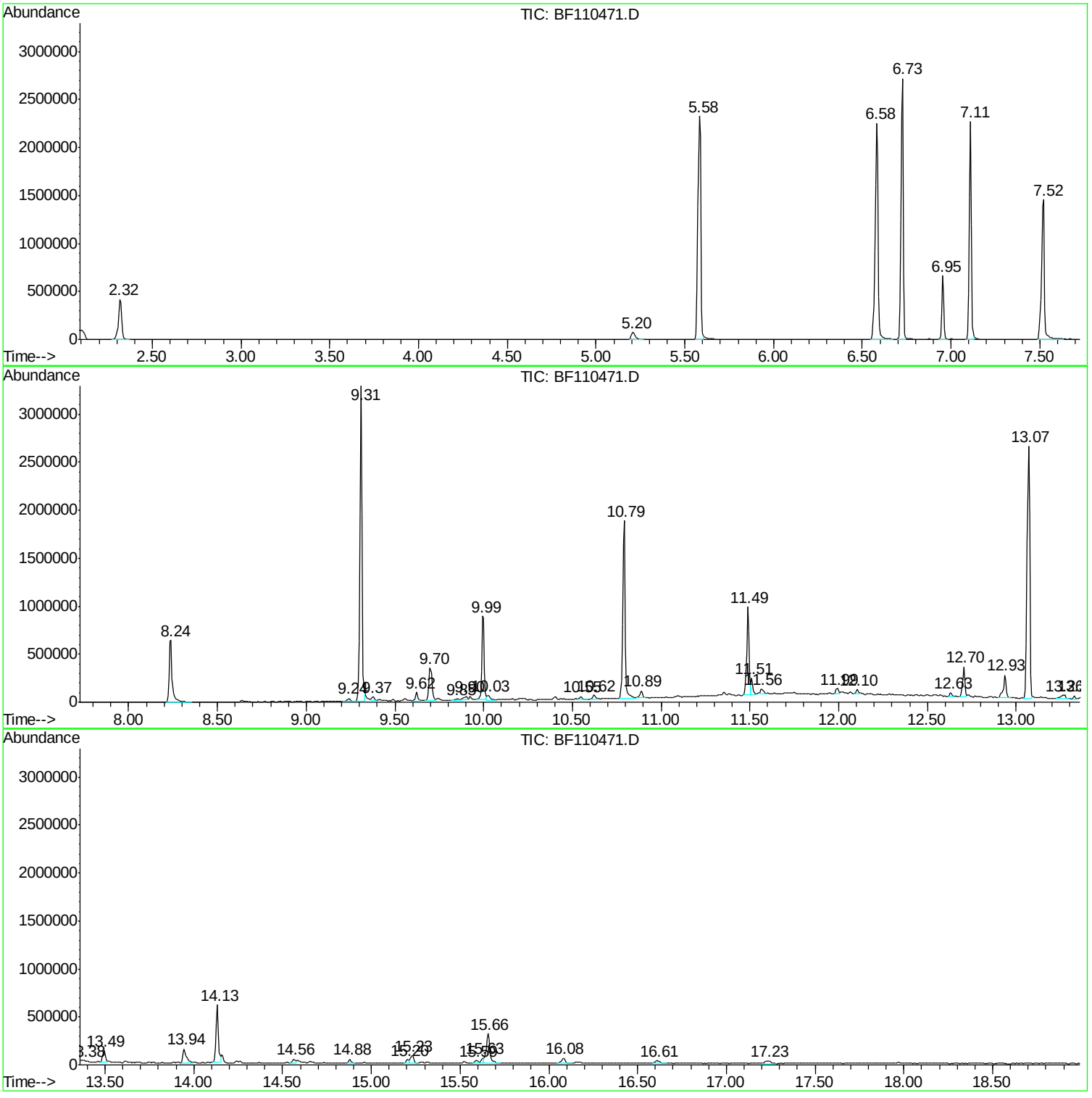
Sample : J5812-25
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP4-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Operator : JU/SJ
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP4-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

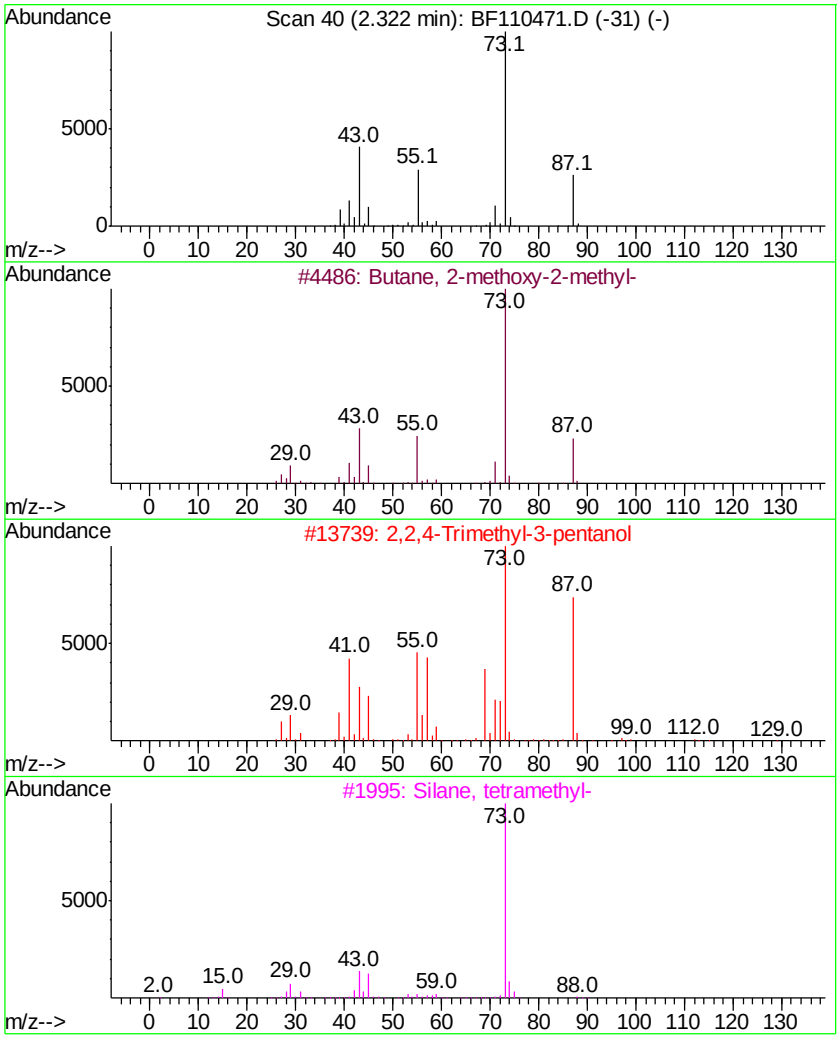
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

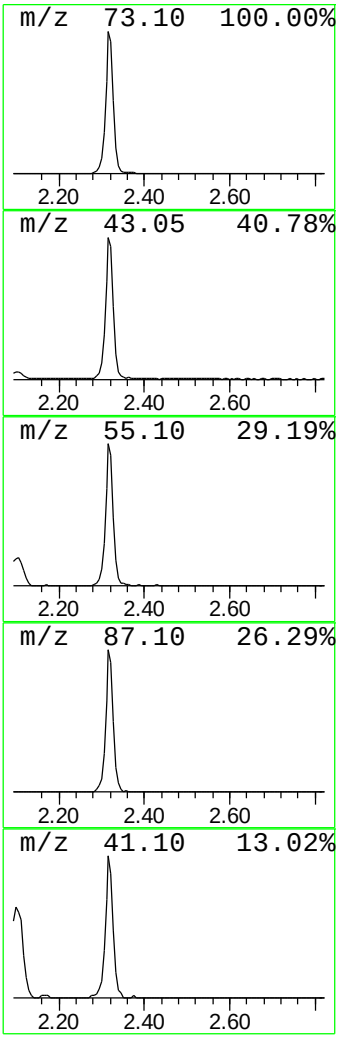
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.32	20.28 ng	562369	1,4-Dichlorobenzene-d4	6.95

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23





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ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP4-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

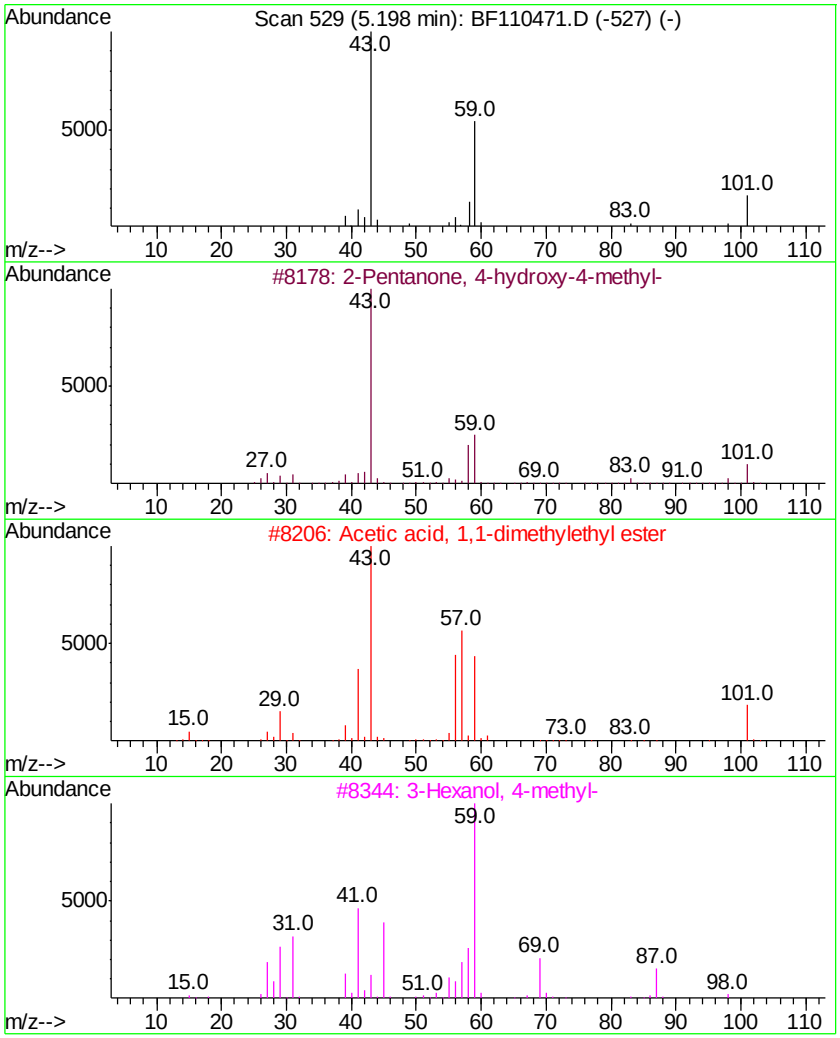
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

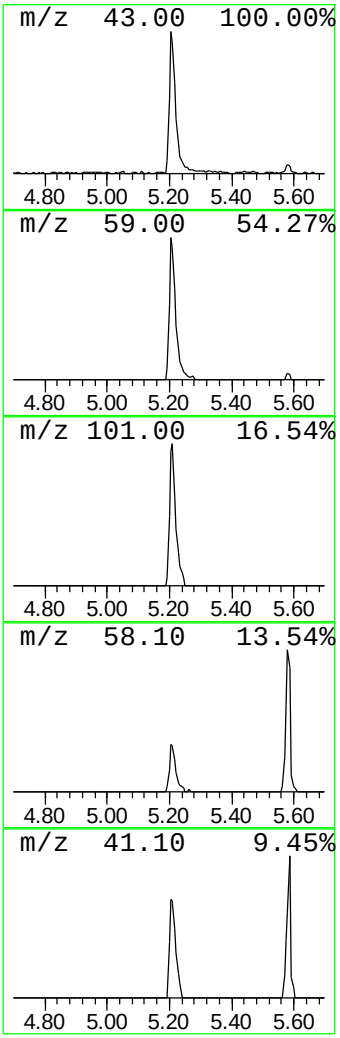
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	3.88 ng	107516	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110518\
Data File : BF110471.D
Acq On : 5 Nov 2018 18:03
Operator : JU/SJ
Sample : J5812-25
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP4-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

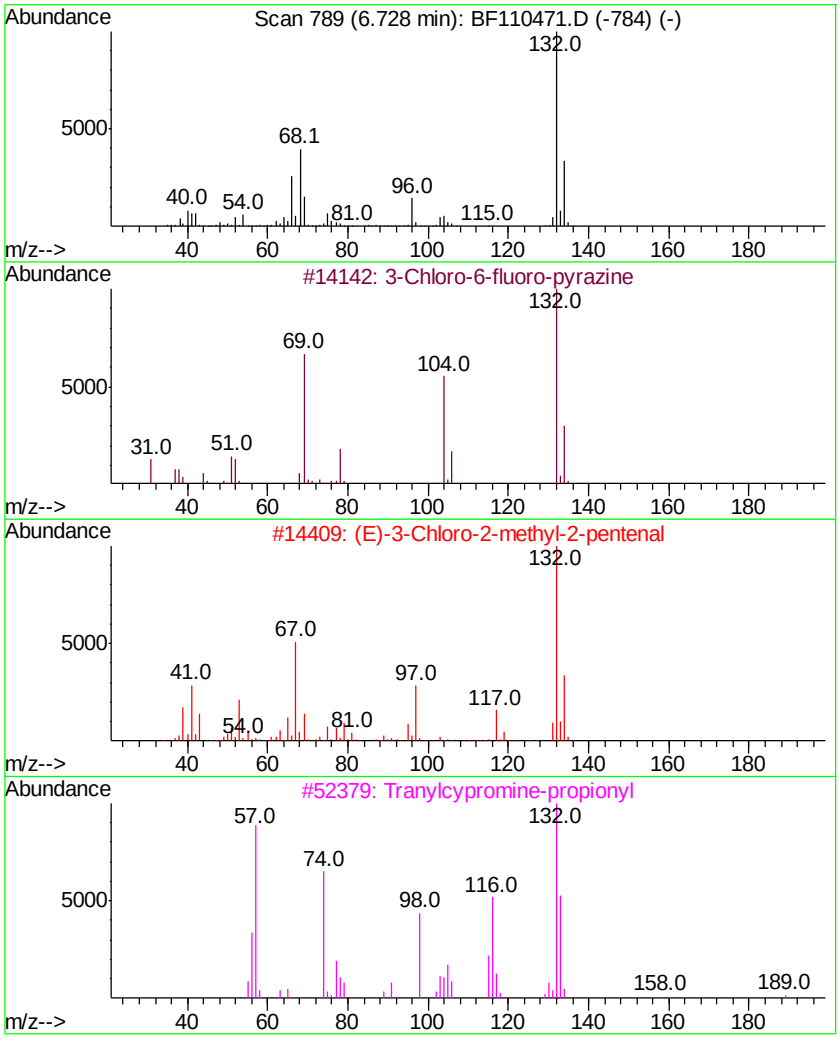
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

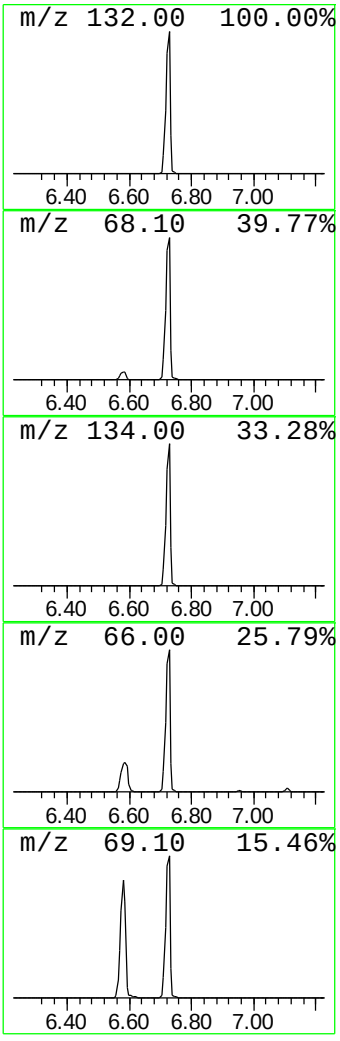
****

Peak Number 3 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	95.03 ng	2635640	1,4-Dichlorobenzene-d4	6.95

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	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP4-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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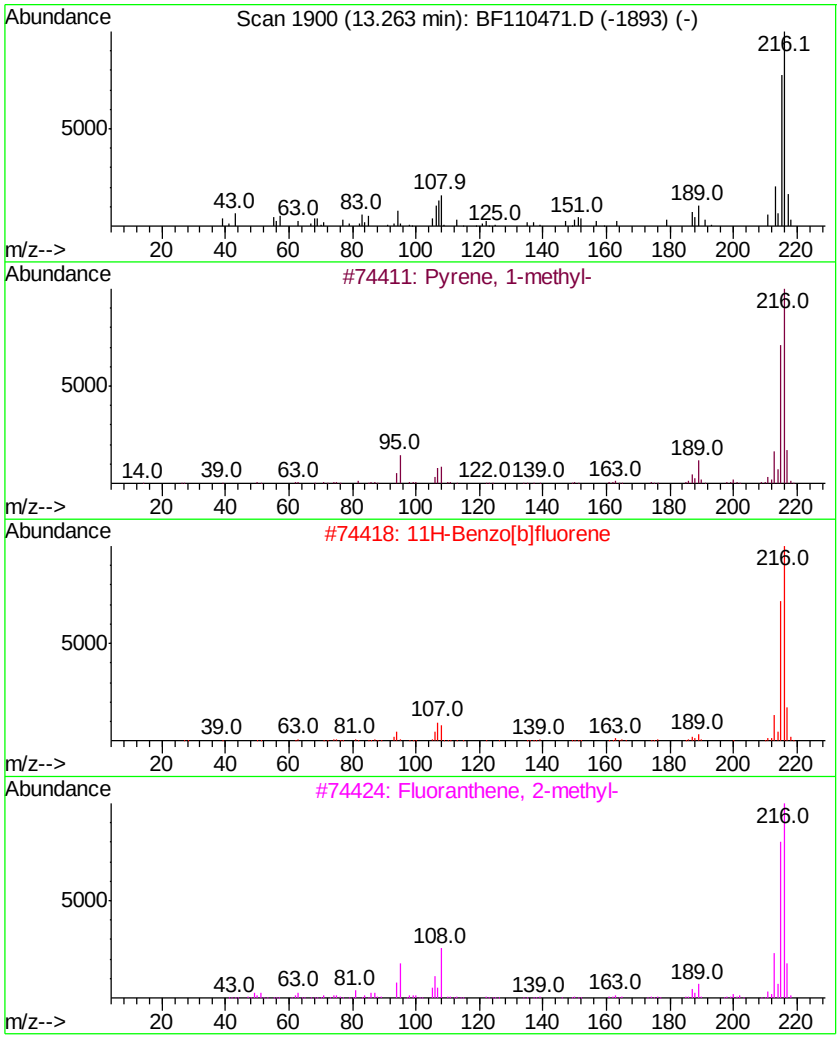
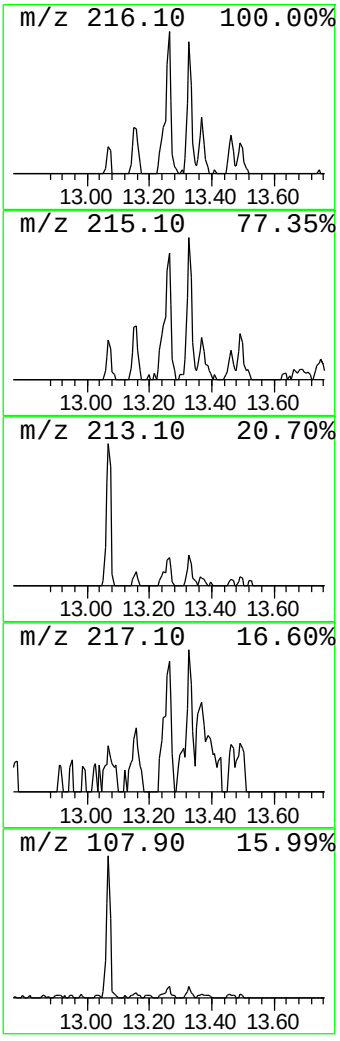
****

Peak Number 5 Pyrene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.26	2.69 ng	81248	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	95
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	94
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87
4	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	87
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	87





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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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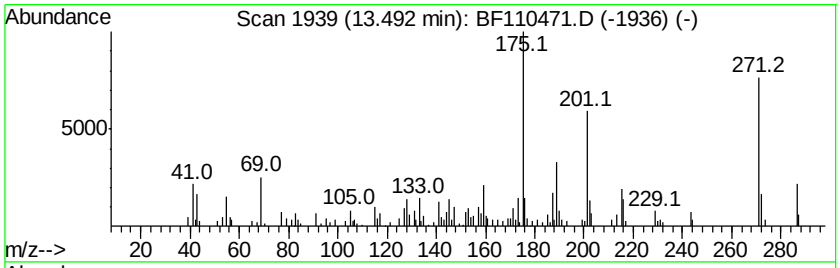
TIC Integration Parameters: LSCINT.P

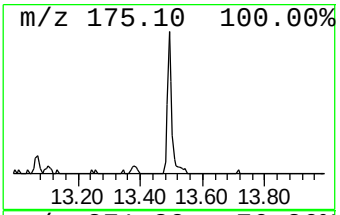
****

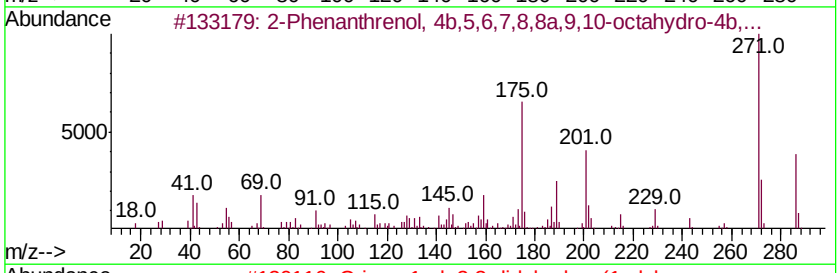
Peak Number 6 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 5

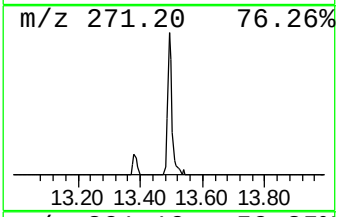
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	3.95 ng	119131	Chrysene-d12	14.13

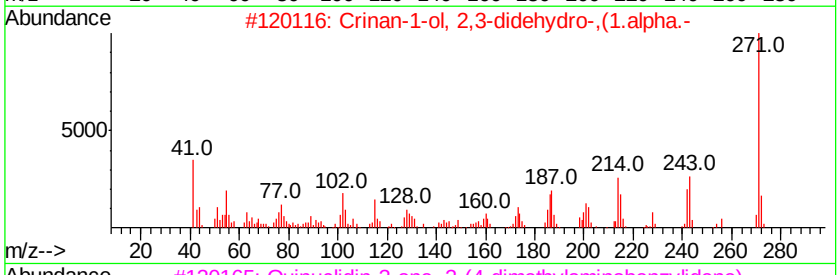
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	55
2	Crinan-1-ol, 2,3-didehydro-,(1.a...	271	C16H17NO3	1000111-31-3	27
3	Quinuclidin-3-one, 2-(4-dimethyl...	271	C16H21N3O	1000266-14-6	25
4	Naphthalene, 1,2,3,4-tetrahydro-...	216	C16H24	002084-69-7	15
5	7-Chloro-5-phenyl-1,3-dihydro-be...	271	C14H10ClN3O	002855-58-5	14

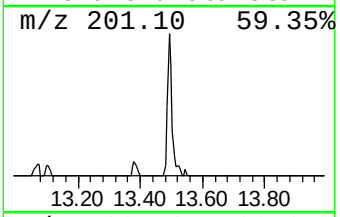


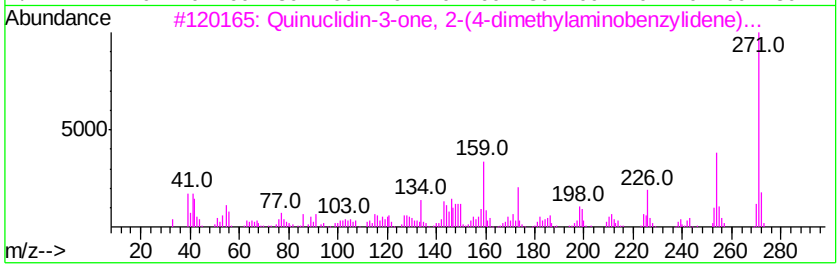


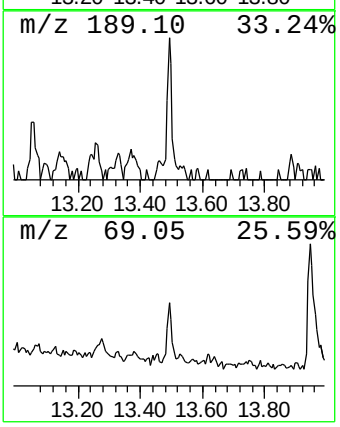












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

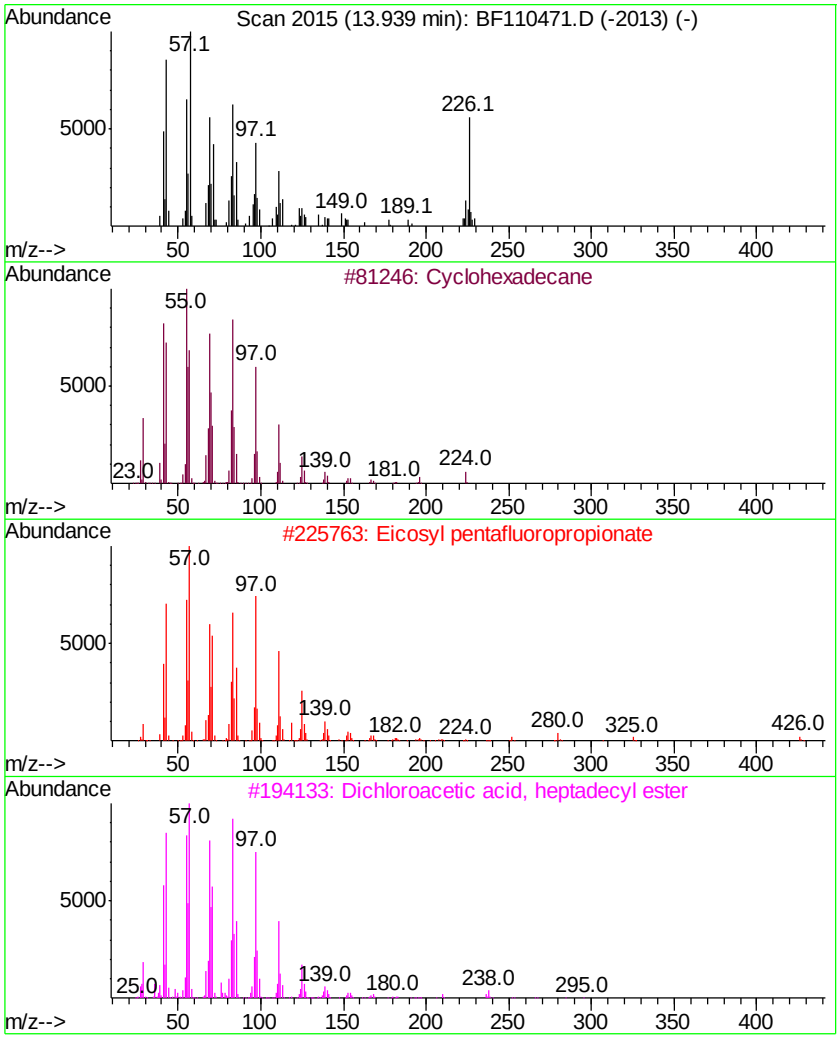
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

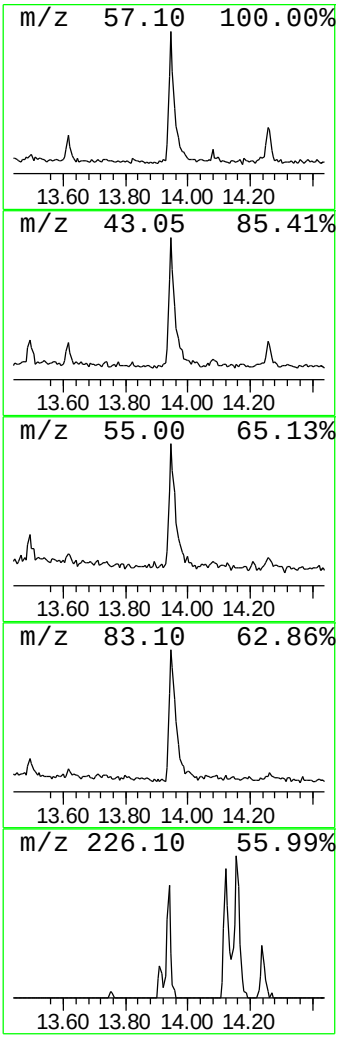
****

Peak Number 7 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	6.67 ng	201333	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	96
2	Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	90
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90
5	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	90





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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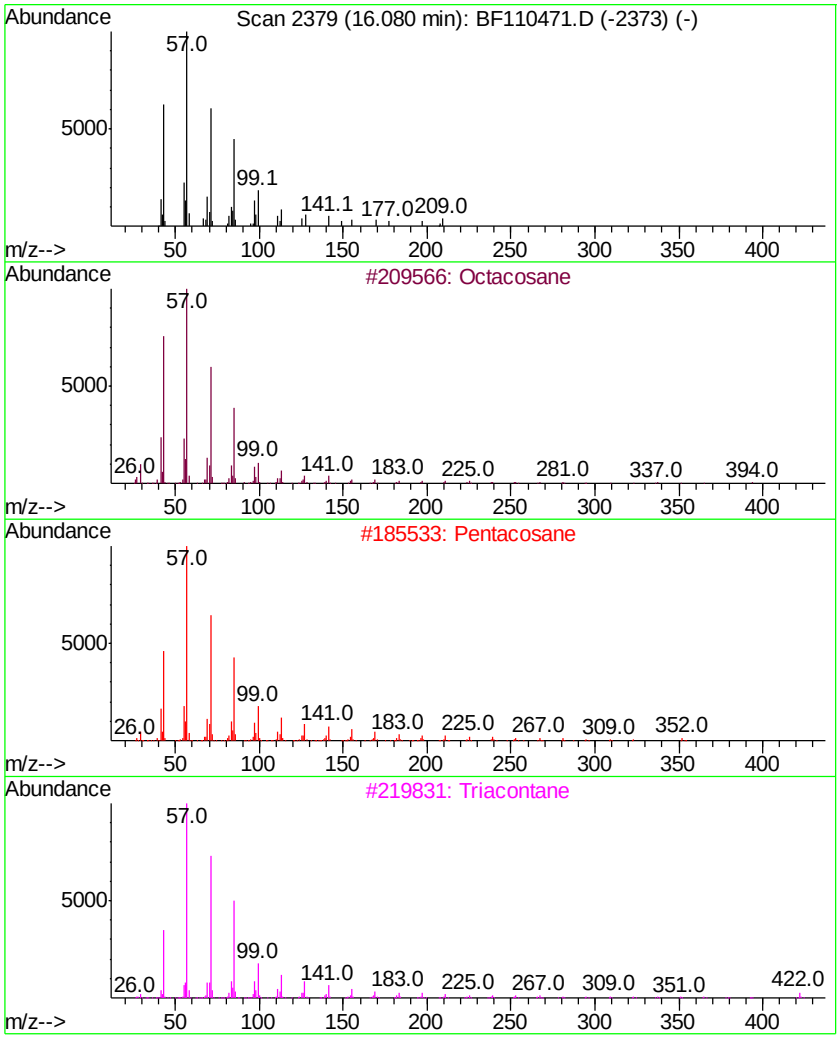
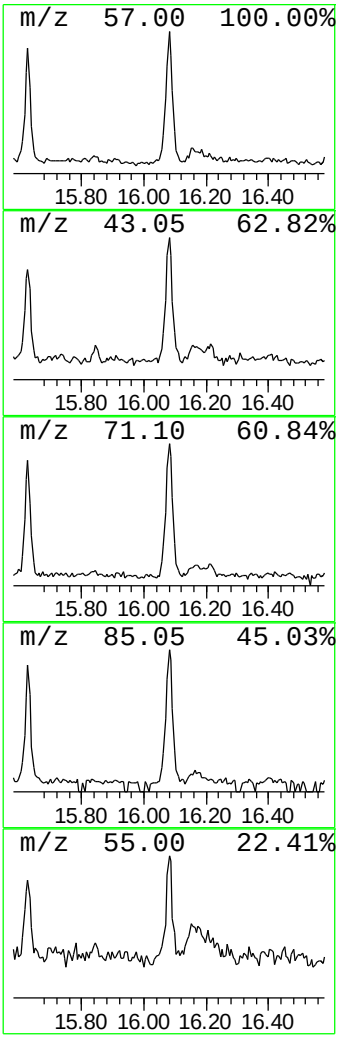
Peak Number 8 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.08	3.83 ng	85972	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Pentacosane	352	C25H52	000629-99-2	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Hentriacontane	437	C31H64	000630-04-6	91
5	Heneicosane	296	C21H44	000629-94-7	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110518\
Data File : BF110471.D
Acq On : 5 Nov 2018 18:03
Operator : JU/SJ
Sample : J5812-25
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP4-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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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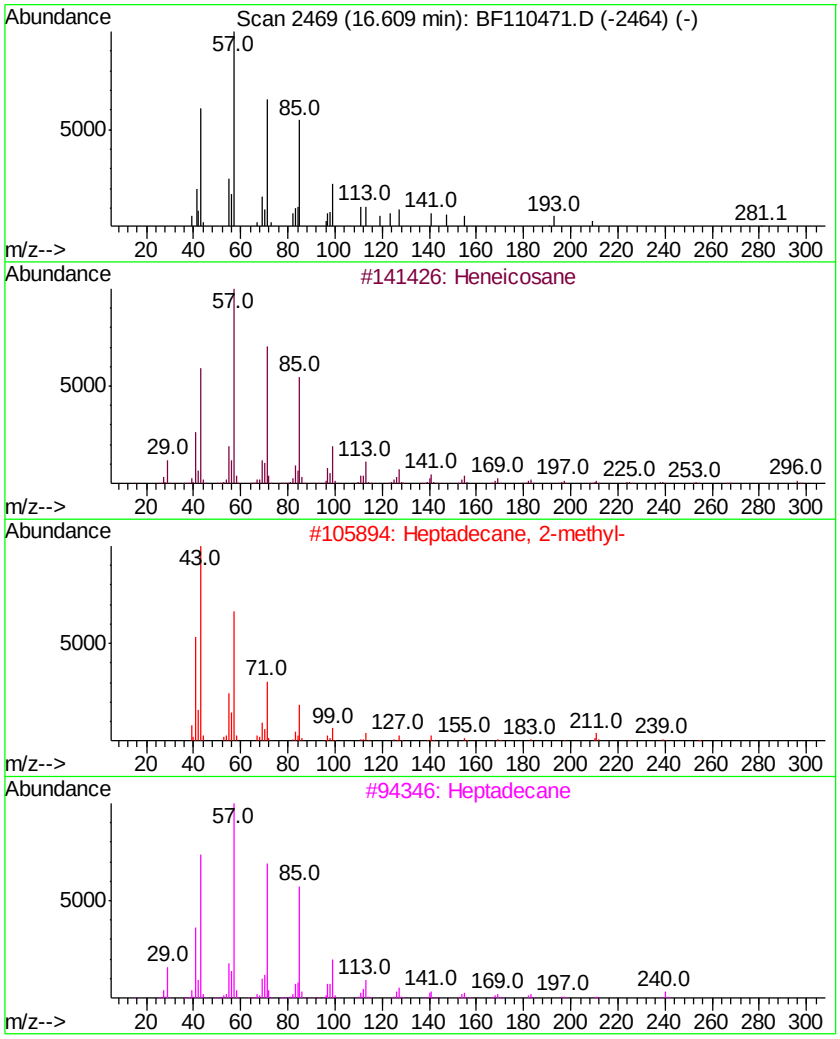
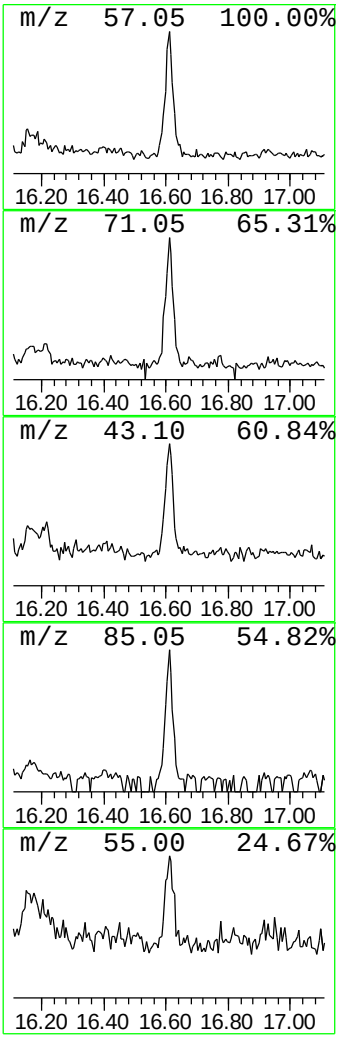
Peak Number 9 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.61	2.25 ng	50540	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	86
3	Heptadecane	240	C17H36	000629-78-7	80
4	Nonahexacontanoic acid	999	C69H138O2	040710-32-5	80
5	2-methyloctacosane	408	C29H60	1000376-72-8	78





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Data File : BF110471.D
Acq On : 5 Nov 2018 18:03
Operator : JU/SJ
Sample : J5812-25
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP4-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

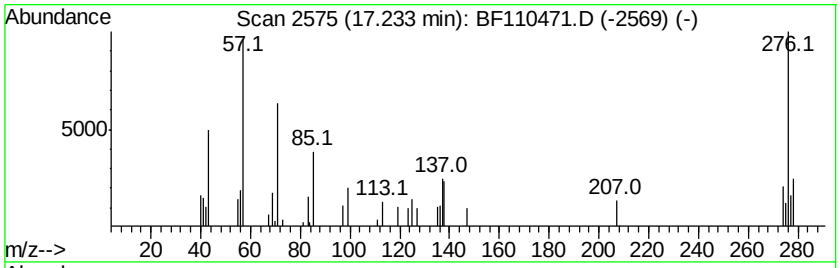
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

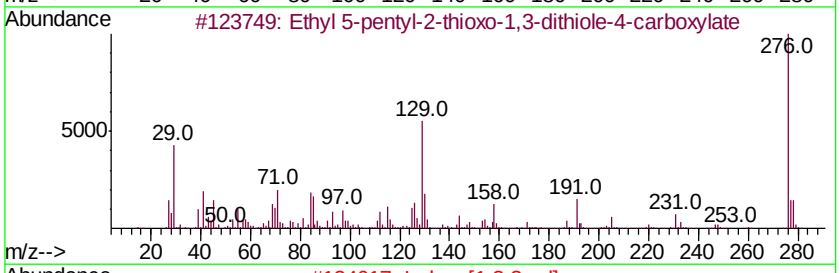
****

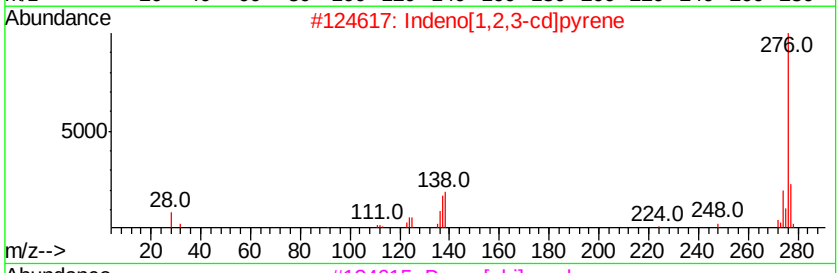
Peak Number 10 Ethyl 5-pentyl-2-thioxo-1,3... Concentration Rank 8

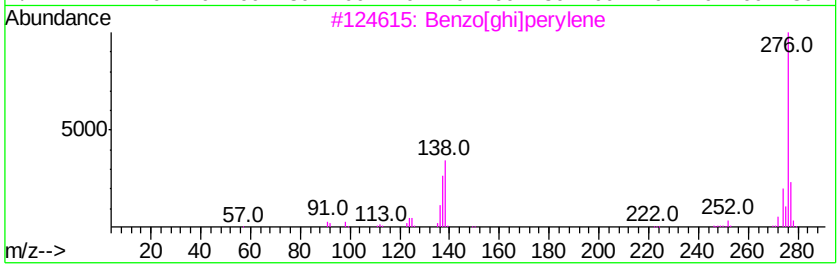
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.23	2.85 ng	63948	Perylene-d12	15.66

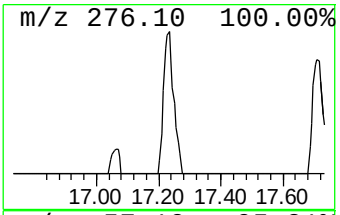
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl 5-pentyl-2-thioxo-1,3-dith...	276	C11H16O2S3	120356-16-3	50
2	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	47
3	Benzo[ghi]perylene	276	C22H12	000191-24-2	43
4	2-{[(4-Chlorophenyl)imino]methyl...	276	C13H9ClN2O3	303215-49-8	35
5	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	35

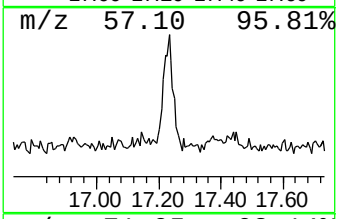


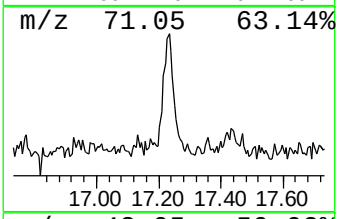


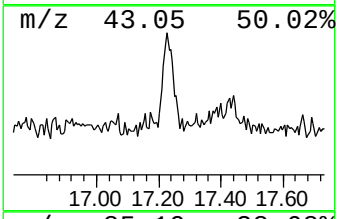


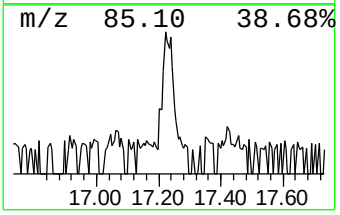












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110518\
Data File : BF110471.D
Acq On : 5 Nov 2018 18:03
Operator : JU/SJ
Sample : J5812-25
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP4-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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-methoxy...	2.32	20.3	ng	562369	1	6.95	554688	20.0
2-Pentanone, 4-hy...	5.20	3.9	ng	107516	1	6.95	554688	20.0
unknown6.73	6.73	95.0	ng	2635640	1	6.95	554688	20.0
Pyrene, 1-methyl-	13.26	2.7	ng	81248	5	14.13	603661	20.0
2-Phenanthrenol, ...	13.49	4.0	ng	119131	5	14.13	603661	20.0
Cyclohexadecane	13.94	6.7	ng	201333	5	14.13	603661	20.0
Octacosane	16.08	3.8	ng	85972	6	15.66	449421	20.0
Heneicosane	16.61	2.3	ng	50540	6	15.66	449421	20.0
Ethyl 5-pentyl-2-...	17.23	2.9	ng	63948	6	15.66	449421	20.0