LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110405.D
Acq On : 2 Nov 2018 12:08
Operator : JU/SJ
Sample : J5741-19
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

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	2.287	29	34	45	rVB	287412	390508	18.45%	2.020%
2	3.593	254	256	269	rBV	14155	36784	1.74%	0.190%
3	5.199	525	529	538	rBV	64492	86355	4.08%	0.447%
4	5.581	589	594	597	rBV	1939689	1735062	81.97%	8.975%
5	6.581	759	764	776	rBV	1818805	1945809	91.93%	10.065%
6	6.722	784	788	792	rBV	1880181	1900980	89.81%	9.833%
7	6.951	824	827	831	rBV	533808	468637	22.14%	2.424%
8	7.110	850	854	857	rBV	1687046	1417309	66.96%	7.331%
9	7.516	918	923	926	rBV	1194538	1151558	54.40%	5.956%
10	7.810	970	973	982	rBV	47487	60890	2.88%	0.315%
11	8.240	1041	1046	1062	rBV	572121	628573	29.70%	3.251%
12	8.451	1078	1082	1088	rBV	55392	63675	3.01%	0.329%
13	8.510	1088	1092	1097	rBV	66093	73781	3.49%	0.382%
14	8.945	1161	1166	1170	rBV2	27783	30171	1.43%	0.156%
15	9.310	1222	1228	1231	rBV	2421403	2116648	100.00%	10.948%
16	9.698	1291	1294	1300	rVB	216446	218668	10.33%	1.131%
17	9.857	1317	1321	1326	rBV	26758	29208	1.38%	0.151%
18	9.998	1341	1345	1352	rVB	662433	674862	31.88%	3.491%
19	10.786	1475	1479	1489	rBV	1234722	1161836	54.89%	6.010%
20	11.486	1594	1598	1601	rBV	661280	618143	29.20%	3.197%
21	11.828	1651	1656	1659	rBV	58967	73325	3.46%	0.379%
22	11.992	1681	1684	1686	rBV	60156	59442	2.81%	0.307%
23	12.028	1686	1690	1694	rVB2	48971	69553	3.29%	0.360%
24	12.539	1774	1777	1780	rBV2	26721	31652	1.50%	0.164%
25	12.704	1802	1805	1809	rBV2	110796	109435	5.17%	0.566%
26	12.933	1840	1844	1850	rVB	124753	145097	6.86%	0.751%
27	13.069	1863	1867	1870	rBV	1888749	1532149	72.39%	7.925%
28	13.257	1893	1899	1901	rBV3	30249	53634	2.53%	0.277%
29	13.616	1957	1960	1963	rBV2	33124	36938	1.75%	0.191%
30	13.945	2013	2016	2021	rBV2	173450	190152	8.98%	0.984%
31	14.133	2043	2048	2051	rBV	513344	516856	24.42%	2.673%
32	14.157	2051	2052	2058	rVB	56041	41600	1.97%	0.215%
33	14.263	2067	2070	2079	rVB4	61186	109910	5.19%	0.569%
34	14.569	2119	2122	2129	rVB2	46884	72387	3.42%	0.374%

LSC Area Percent Report

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Operator : JU/SJ
Sample : J5741-19
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

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	14.886	2171	2176	2179	rBV2	76980	102043	4.82%	0.528%
36	14.963	2187	2189	2193	rVB3	26392	27663	1.31%	0.143%
37	15.204	2226	2230	2232	rBV	41478	56091	2.65%	0.290%
38	15.233	2232	2235	2241	rVB2	97656	120727	5.70%	0.624%
39	15.521	2280	2284	2288	rVB	39983	54731	2.59%	0.283%
40	15.586	2291	2295	2299	rVV2	53755	77666	3.67%	0.402%
41	15.657	2299	2307	2322	rVB2	371935	632116	29.86%	3.270%
42	16.092	2375	2381	2387	rBV	77770	123521	5.84%	0.639%
43	16.163	2389	2393	2398	rVB4	38993	60957	2.88%	0.315%
44	16.621	2467	2471	2478	rVB	51911	89268	4.22%	0.462%
45	17.221	2567	2573	2582	rVB3	27509	87560	4.14%	0.453%
46	17.692	2648	2653	2661	rVB2	23430	48891	2.31%	0.253%

Sum of corrected areas: 19332821

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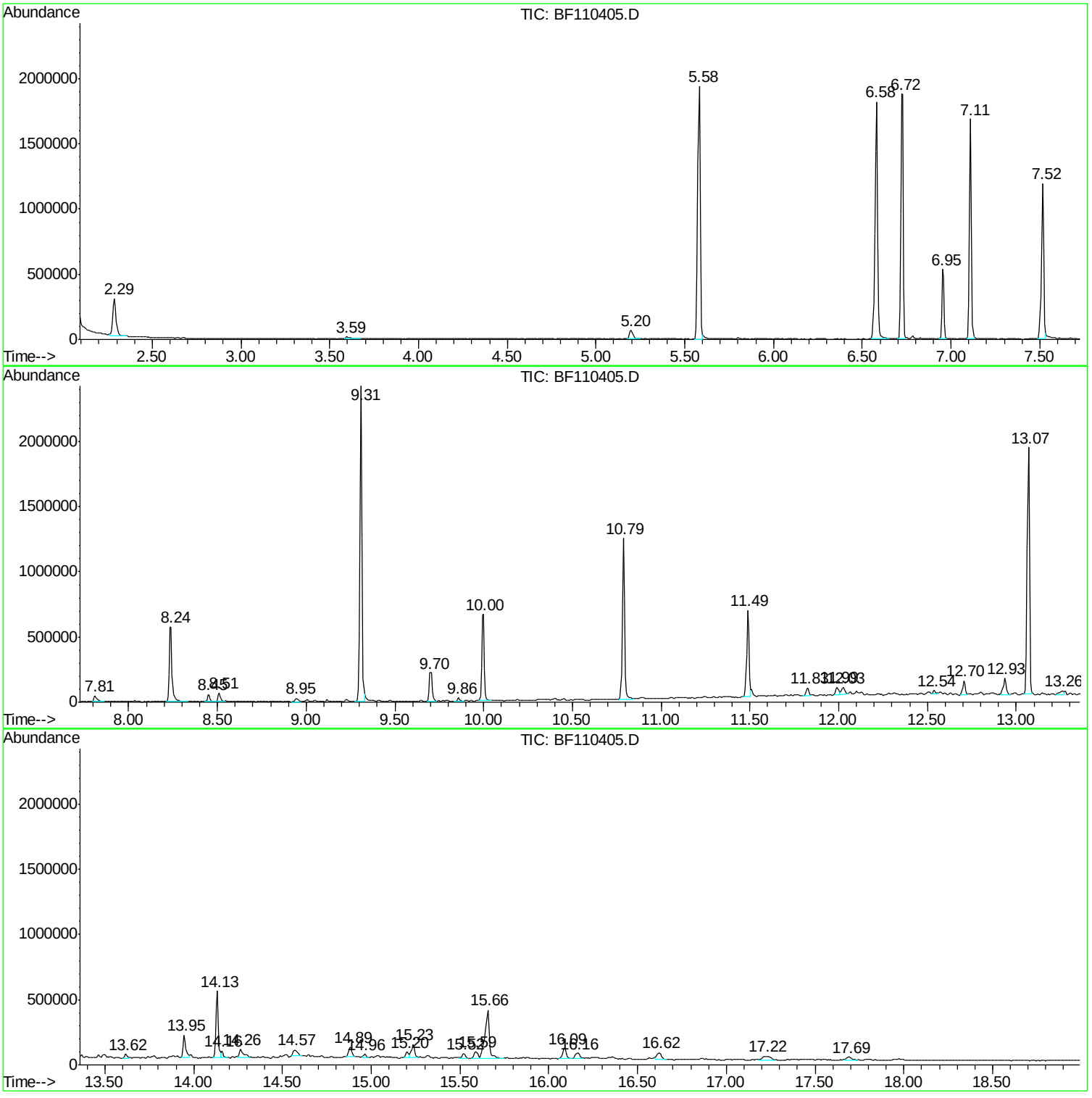
Instrument : BNA_F
ClientSampleId : TP-5

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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Instrument : BNA_F
ClientSampleId : TP-5

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

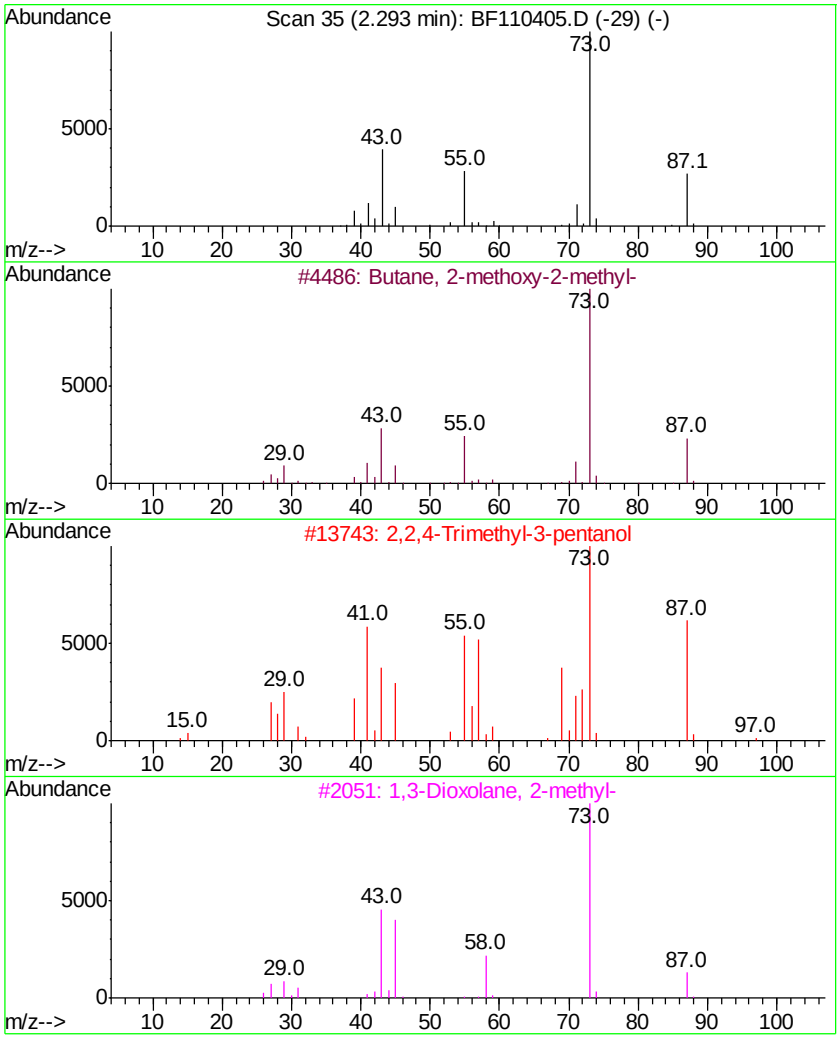
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

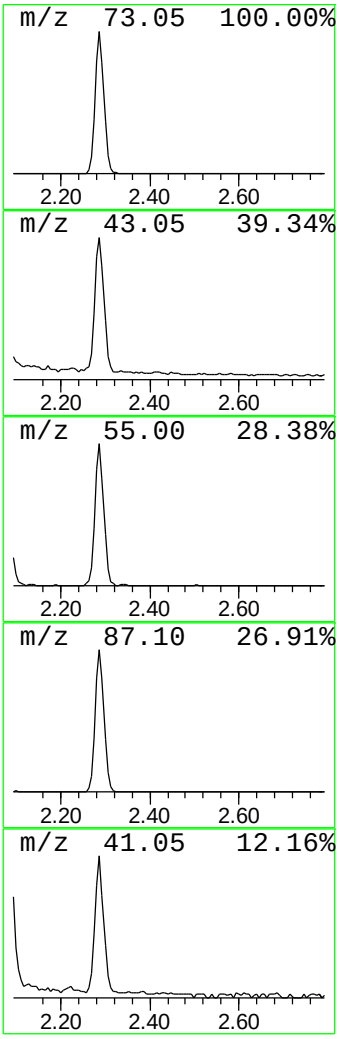
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.29	16.67 ng	390508	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	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10





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ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

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

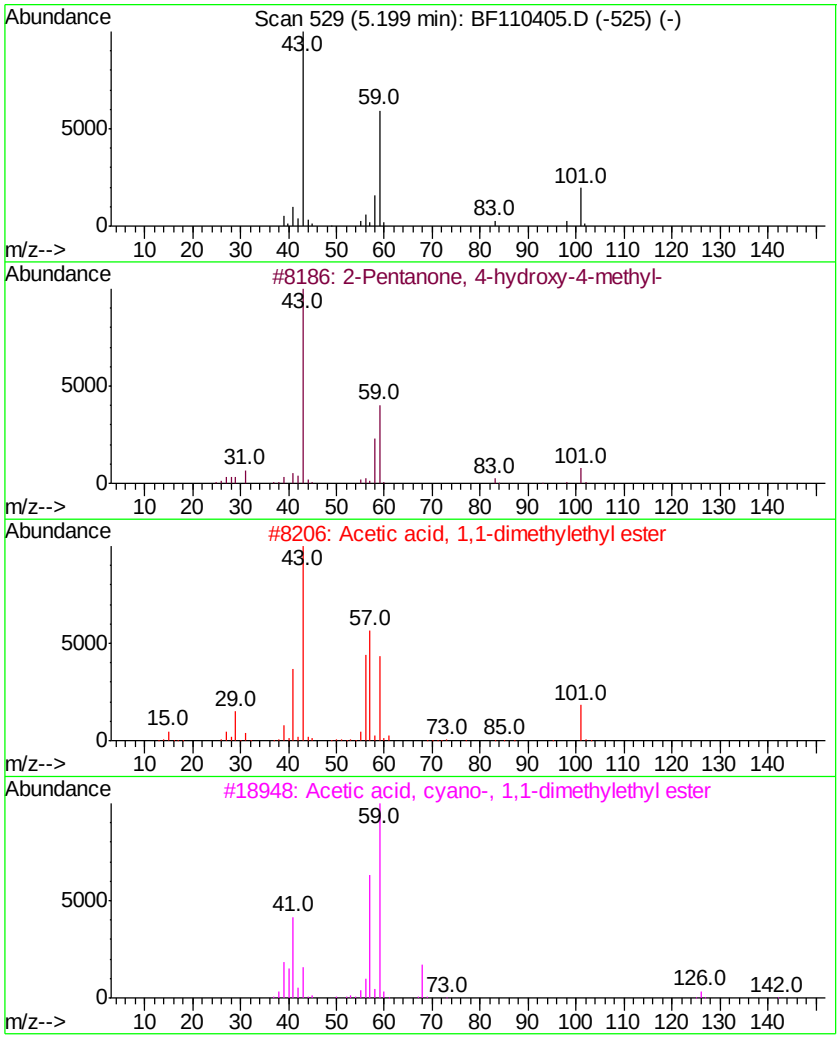
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

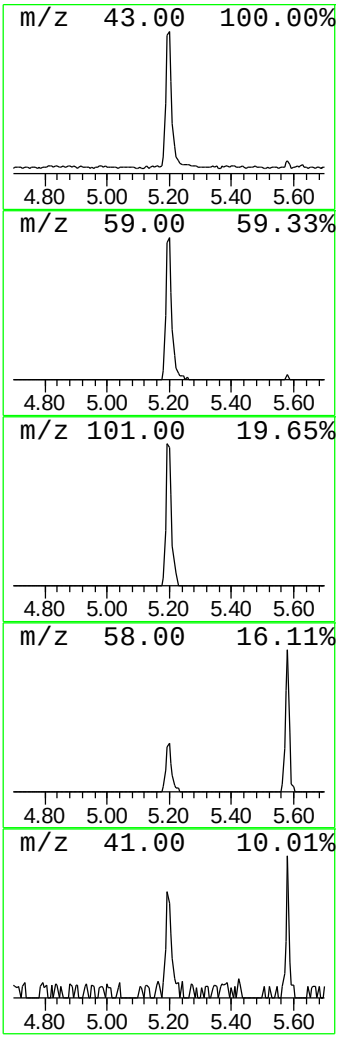
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	3.69 ng	86355	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	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

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

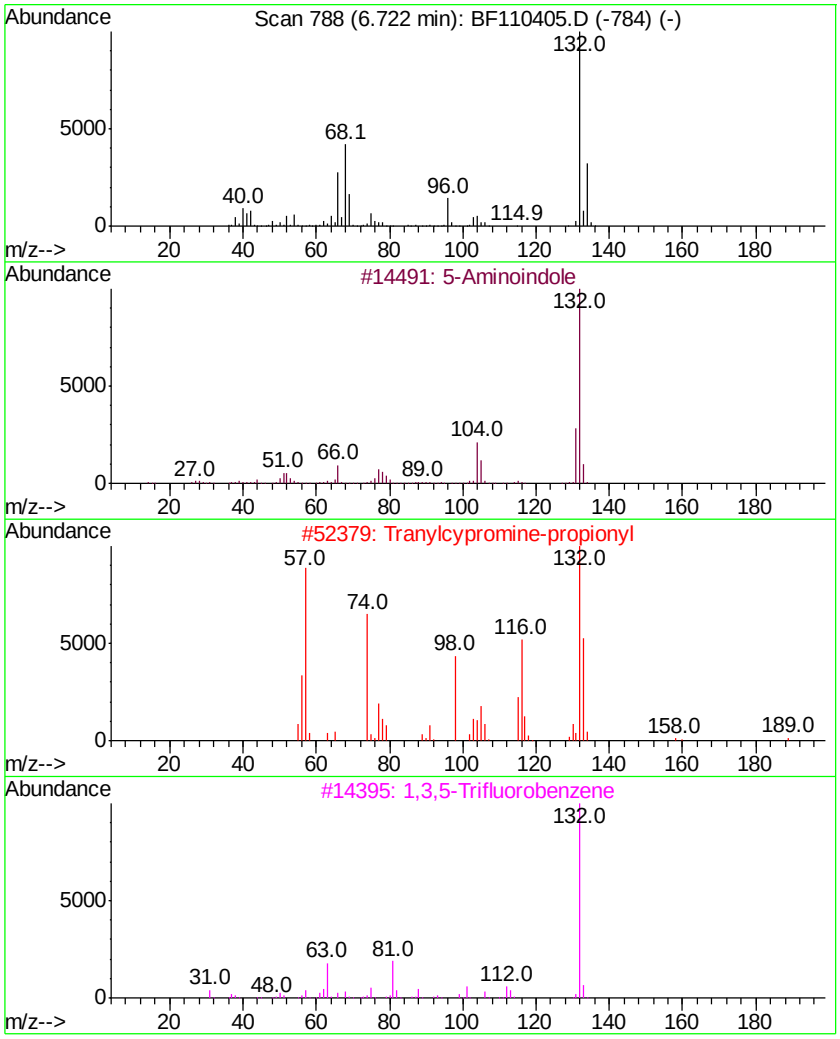
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

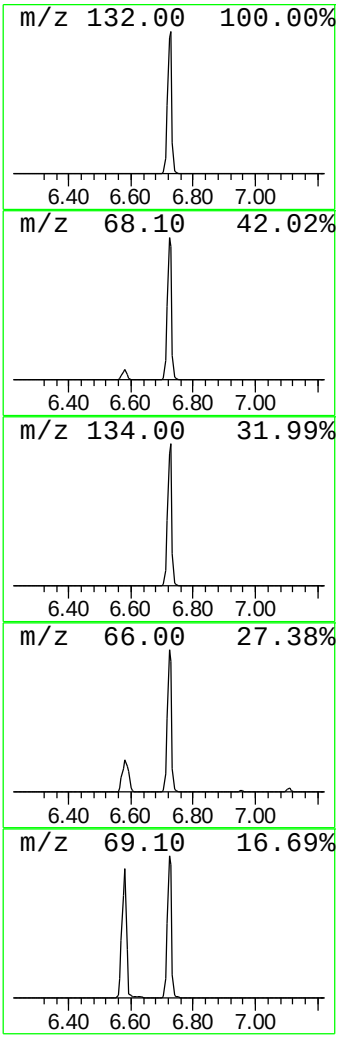
****

Peak Number 3 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	81.13 ng	1900980	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

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

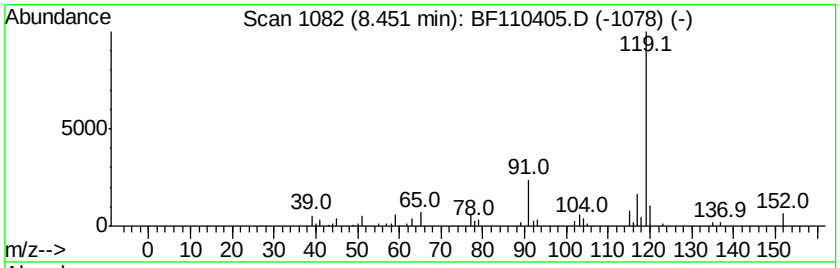
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

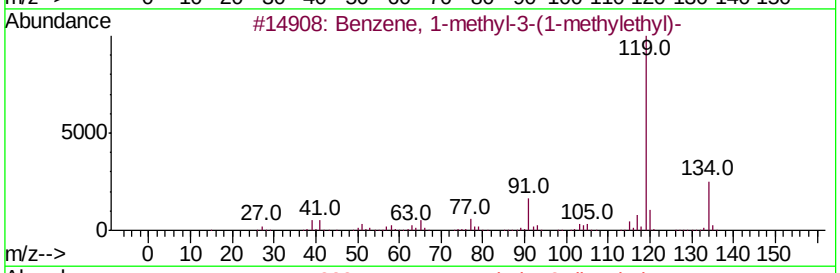
****

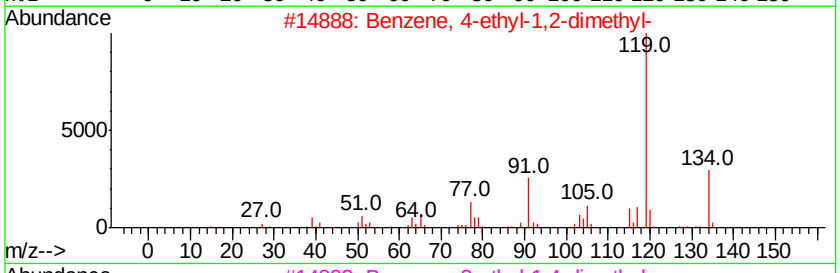
Peak Number 5 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 15

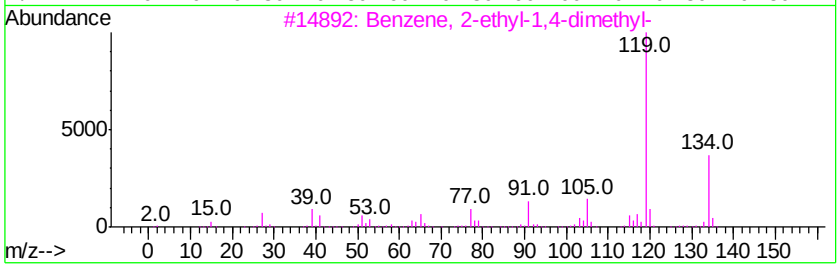
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.45	2.03 ng	63675	Naphthalene-d8	8.24

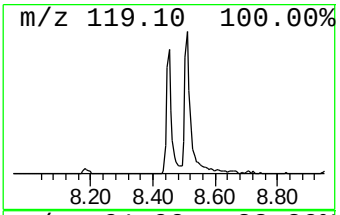
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	80
2	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	72
3	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	72
4	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	72
5	o-Cymene	134	C10H14	000527-84-4	72

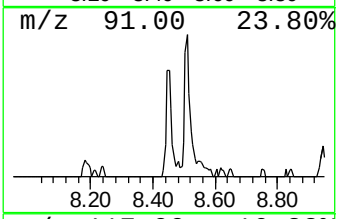


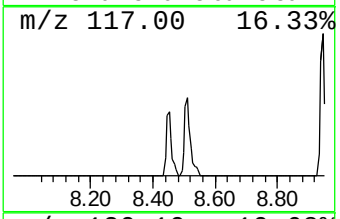


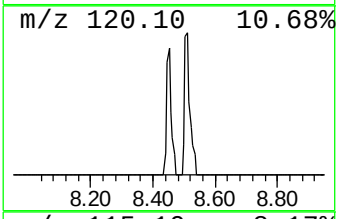


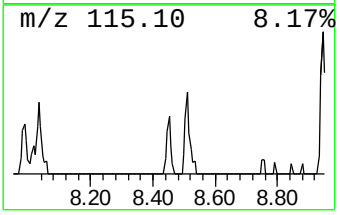












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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

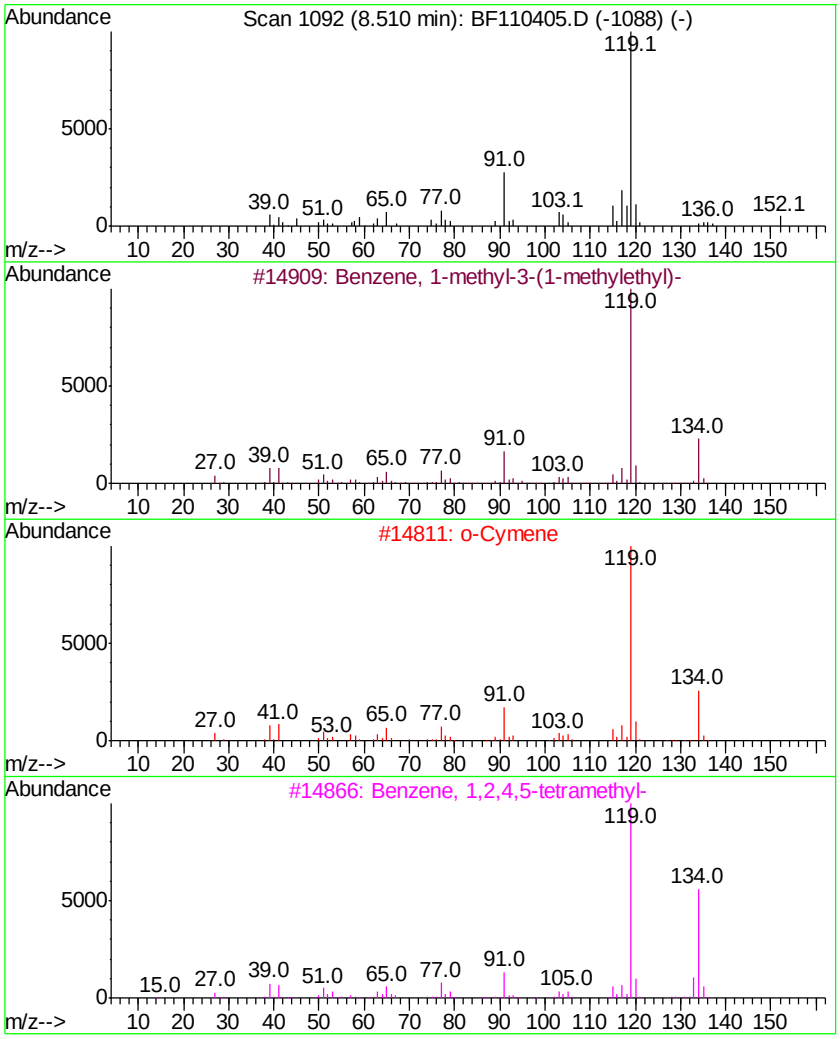
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

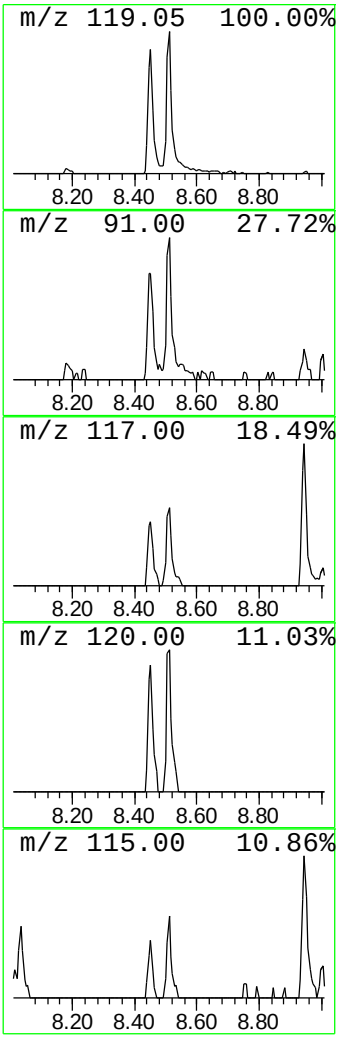
****

Peak Number 6 Benzene, 1-methyl-3-(1-meth... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.51	2.35 ng	73781	Naphthalene-d8	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	83
2	o-Cymene	134	C10H14	000527-84-4	81
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	72
4	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	72
5	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	64





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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

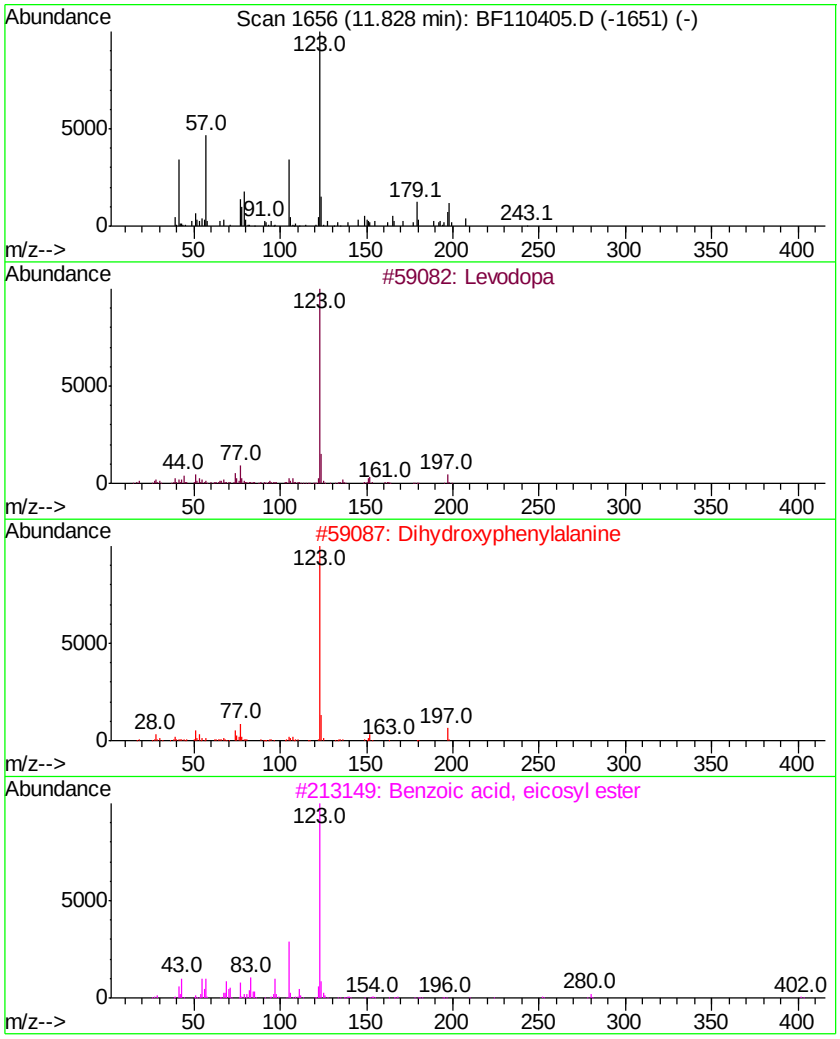
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

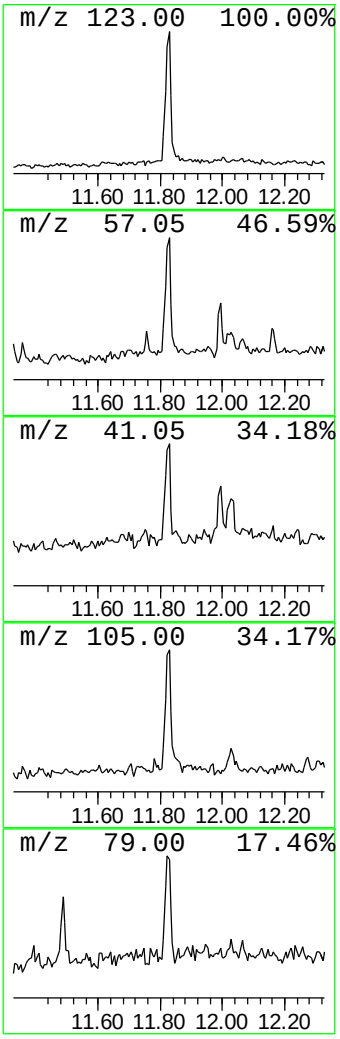
****

Peak Number 7 unknown11.83 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.83	2.37 ng	73325	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Levodopa	197	C9H11NO4	000059-92-7	47
2	Dihydroxyphenylalanine	197	C9H11NO4	000063-84-3	47
3	Benzoic acid, eicosyl ester	402	C27H46O2	1000340-23-3	42
4	Glycine, N-(2-fluorobenzoyl)-, i...	281	C15H20FNO3	1000314-47-8	40
5	6-Ethoxycarbonylpyridine-3-carbo...	195	C9H9NO4	017874-78-1	38





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Misc :
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Instrument : BNA_F
ClientSampleId : TP-5

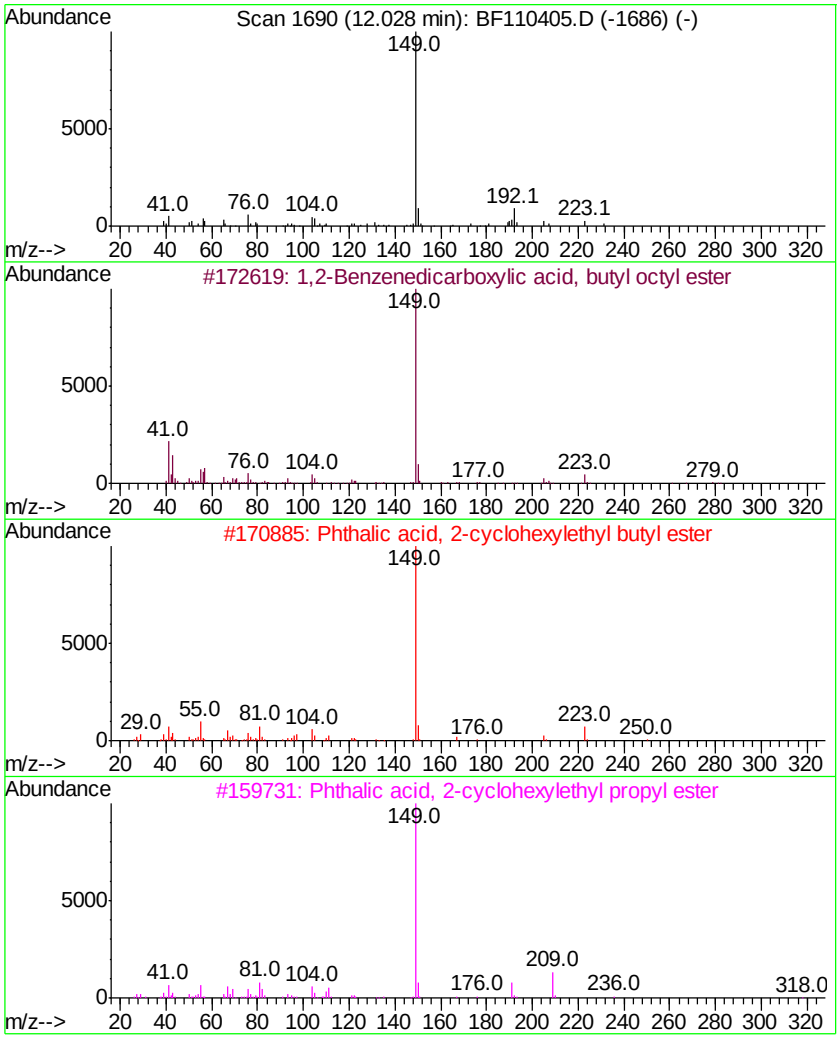
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

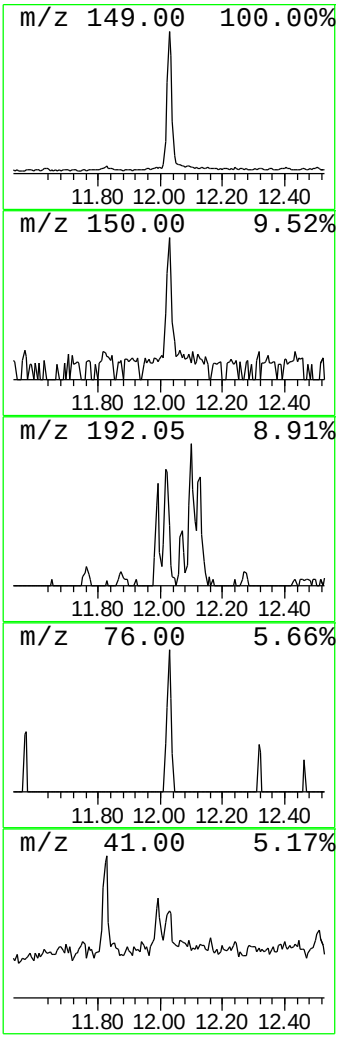
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1,2-Benzenedicarboxylic aci... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.03	2.25 ng	69553	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000084-78-6	72
2	Phthalic acid, 2-cyclohexylethyl...	332	C20H28O4	1000309-08-4	72
3	Phthalic acid, 2-cyclohexylethyl...	318	C19H26O4	1000309-08-5	72
4	Phthalic acid, butyl hexyl ester	306	C18H26O4	1000308-99-5	72
5	1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000085-69-8	72





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110405.D
Acq On : 2 Nov 2018 12:08
Operator : JU/SJ
Sample : J5741-19
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

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

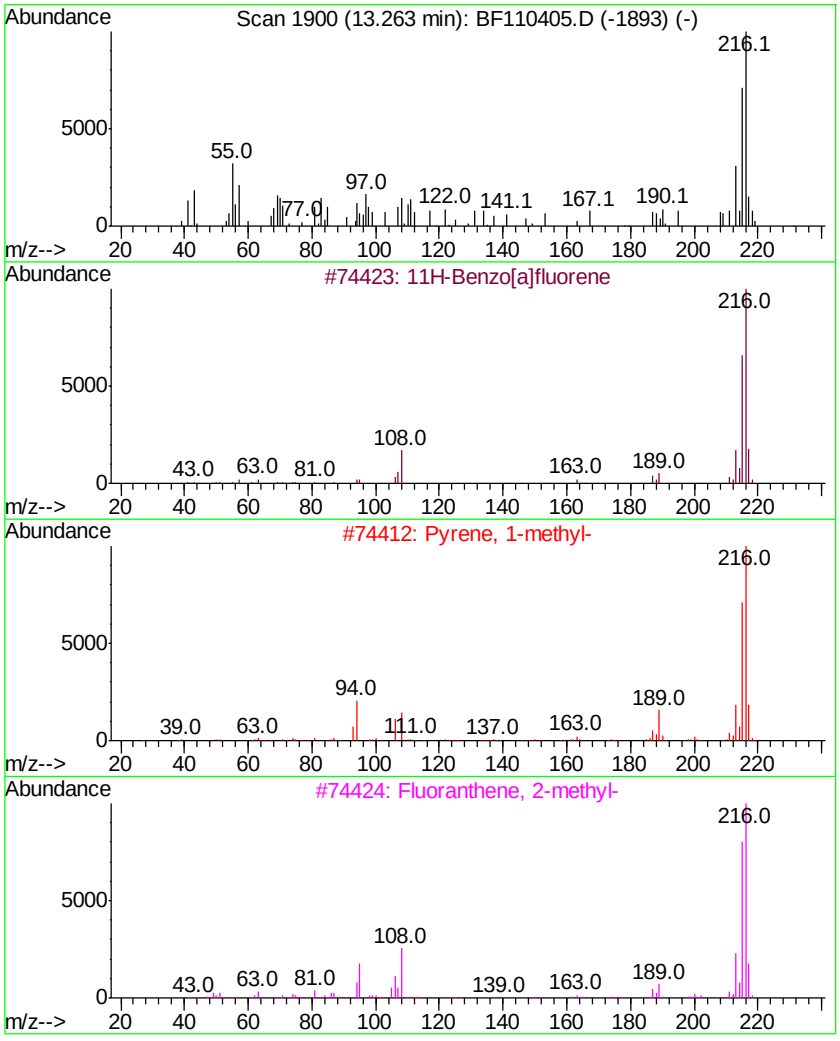
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

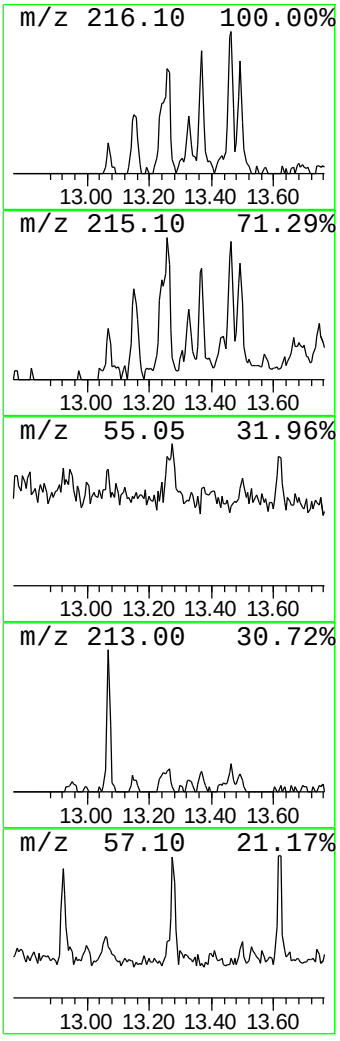
****

Peak Number 9 11H-Benzo[a]fluorene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.26	2.08 ng	53634	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	76
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	72
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	68
4	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	59
5	Benzoic acid, 3-(3,5-dimethyl-1-...	216	C12H12N2O2	312531-88-7	58





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Acq On : 2 Nov 2018 12:08
Operator : JU/SJ
Sample : J5741-19
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

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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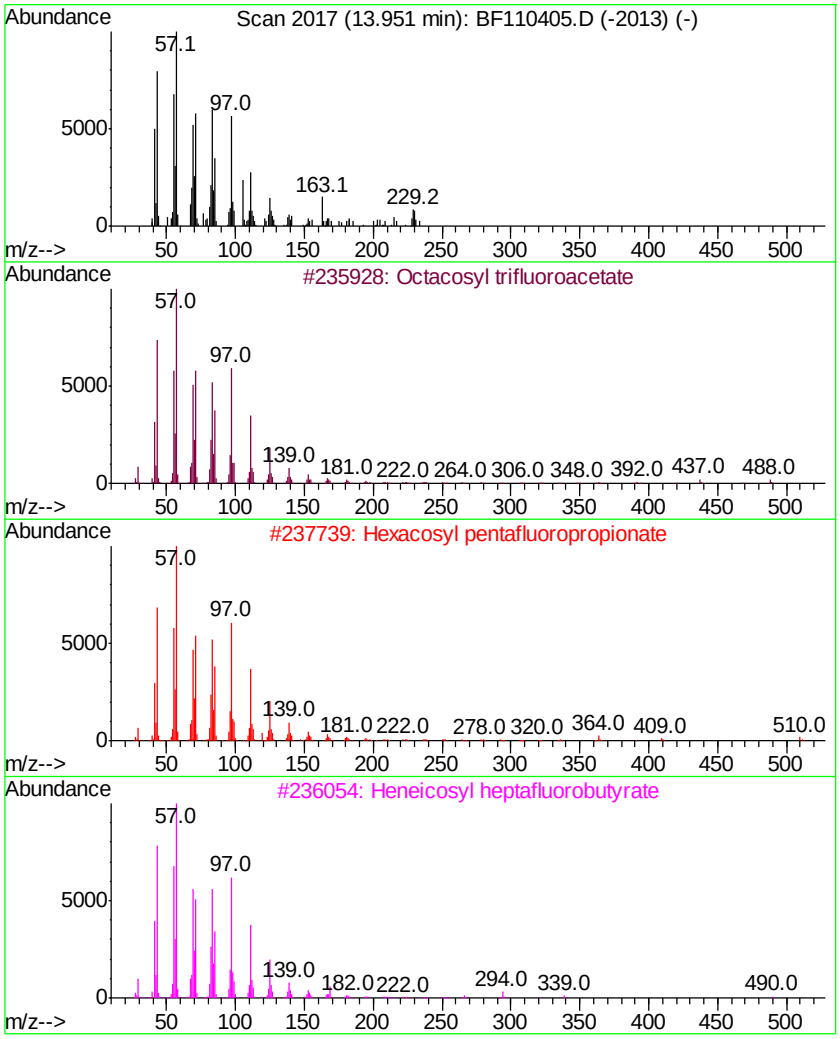
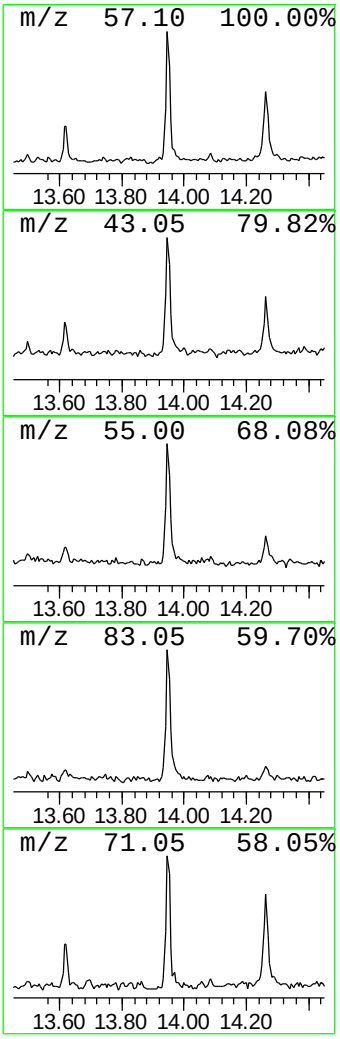
Peak Number 10 Octacosyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	7.36 ng	190152	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	90
2	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	87
3	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	87
4	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	87
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87





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Sample : J5741-19
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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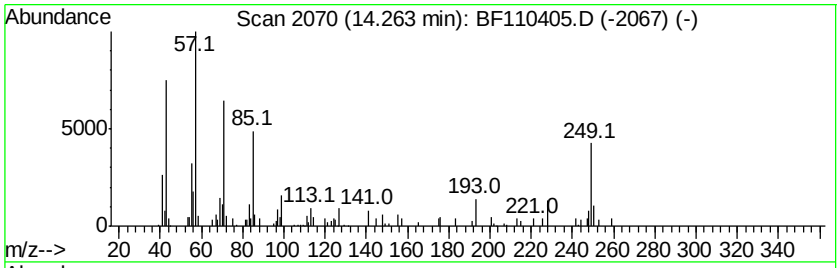
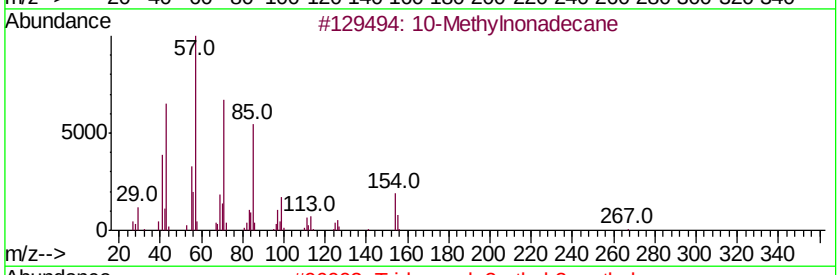
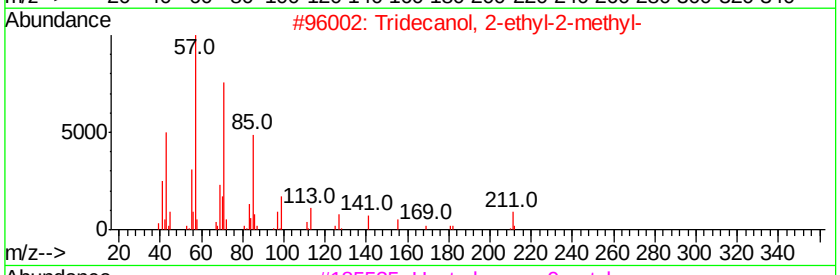
Peak Number 11 unknown14.26 Concentration Rank 5

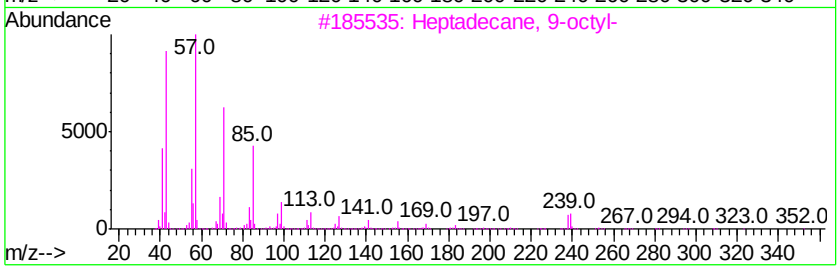
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.26	4.25 ng	109910	Chrysene-d12	14.13

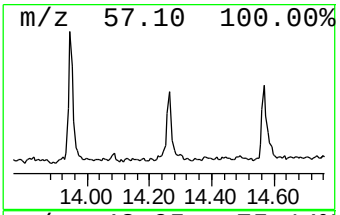
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Methylnonadecane	282	C20H42	056862-62-5	46
2	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	45
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	45
4	Octacosane	394	C28H58	000630-02-4	45
5	Tetracosane	338	C24H50	000646-31-1	45

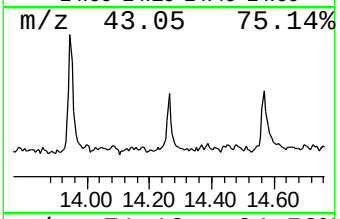


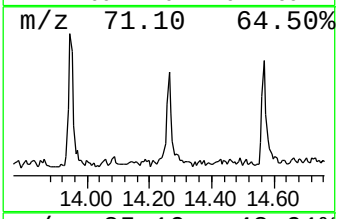


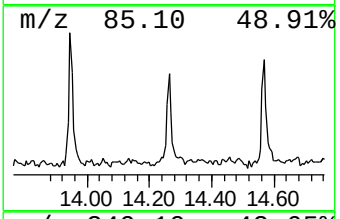


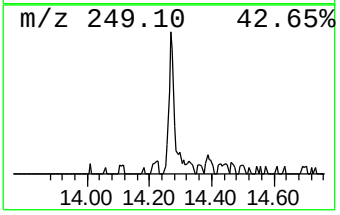












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Sample : J5741-19
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

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

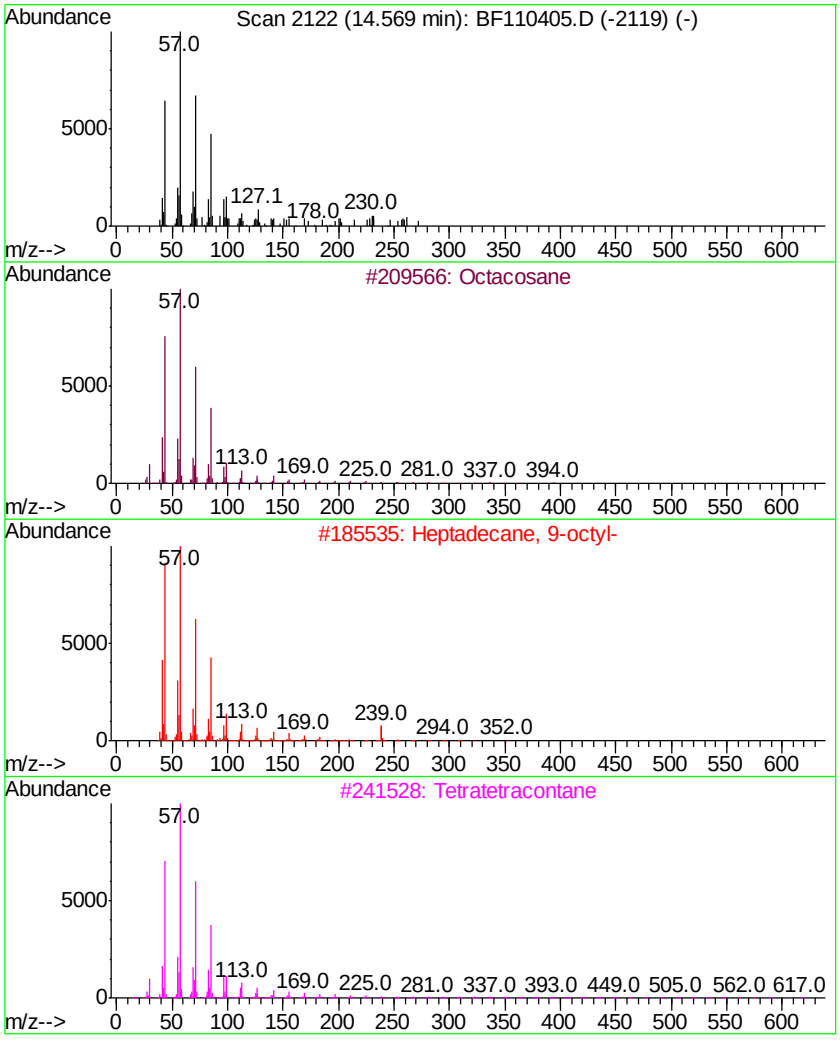
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

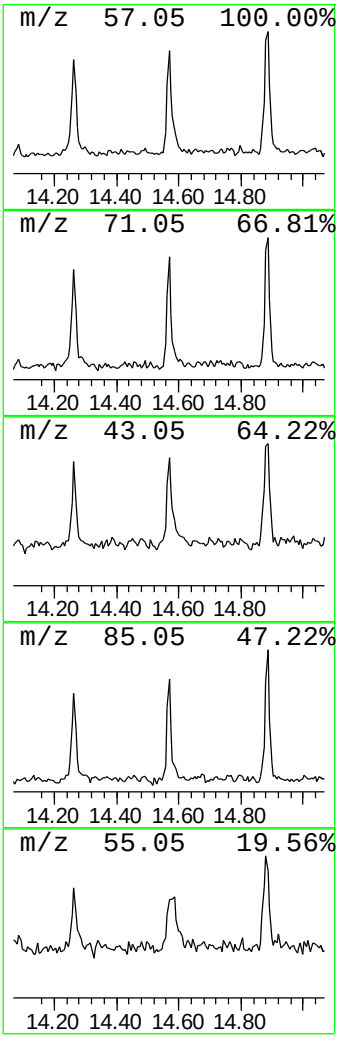
****

Peak Number 12 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	2.80 ng	72387	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	74
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	74
3	Tetratetracontane	619	C44H90	007098-22-8	72
4	Tetracosane	338	C24H50	000646-31-1	72
5	Heptadecane	240	C17H36	000629-78-7	72





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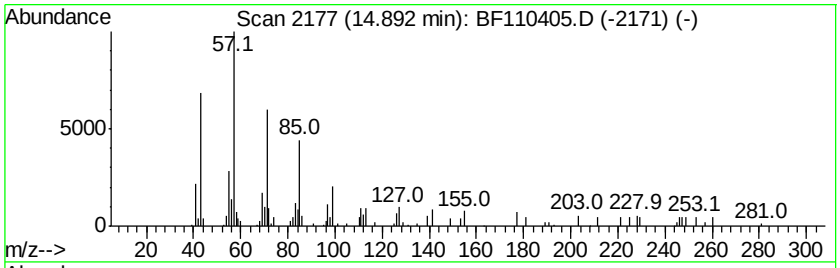
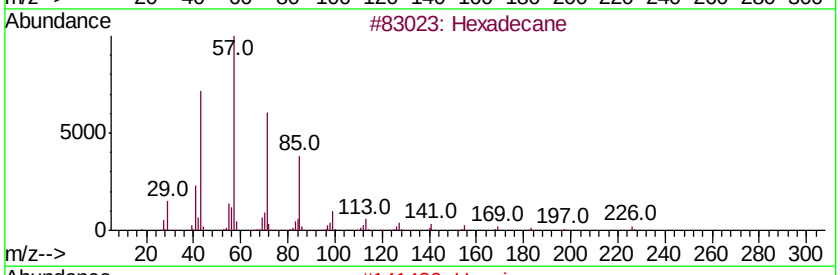
****

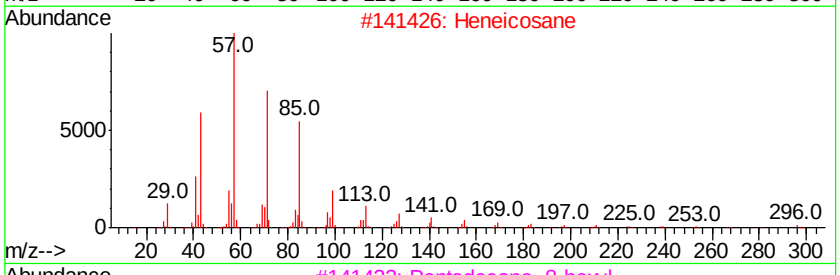
Peak Number 13 Hexadecane Concentration Rank 6

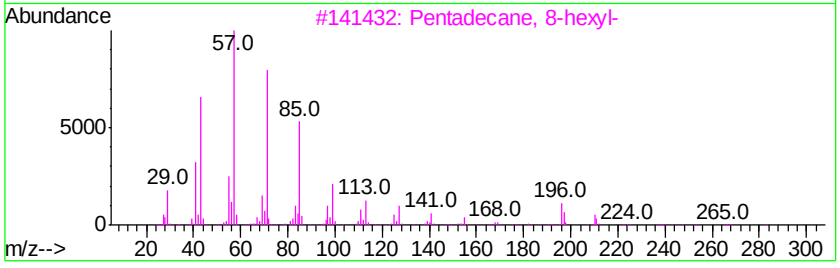
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	3.95 ng	102043	Chrysene-d12	14.13

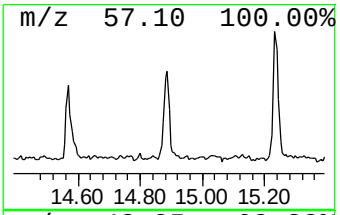
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	93
2	Heneicosane	296	C21H44	000629-94-7	87
3	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	80
4	Heptadecane	240	C17H36	000629-78-7	80
5	2-methyloctacosane	408	C29H60	1000376-72-8	74

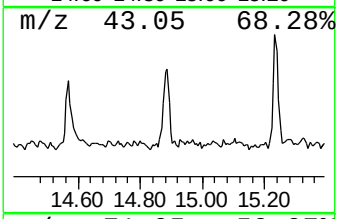


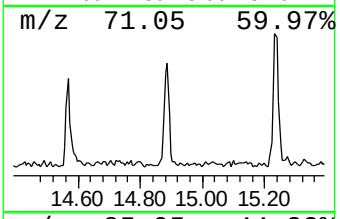


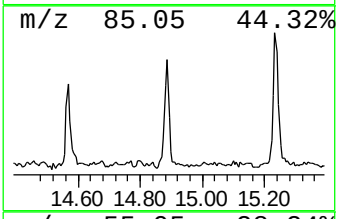


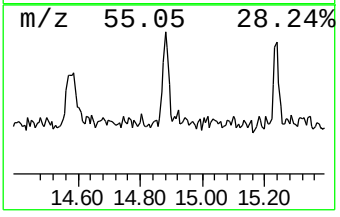












Library Search Compound Report

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Data File : BF110405.D
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Operator : JU/SJ
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

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

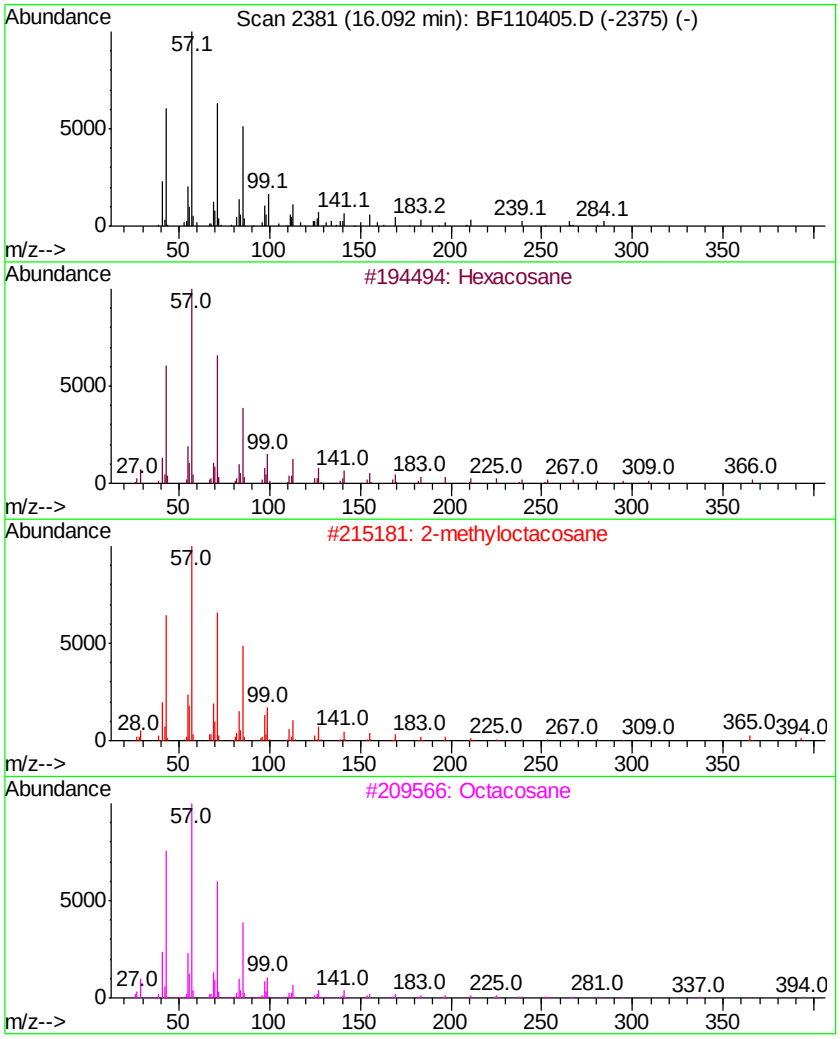
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

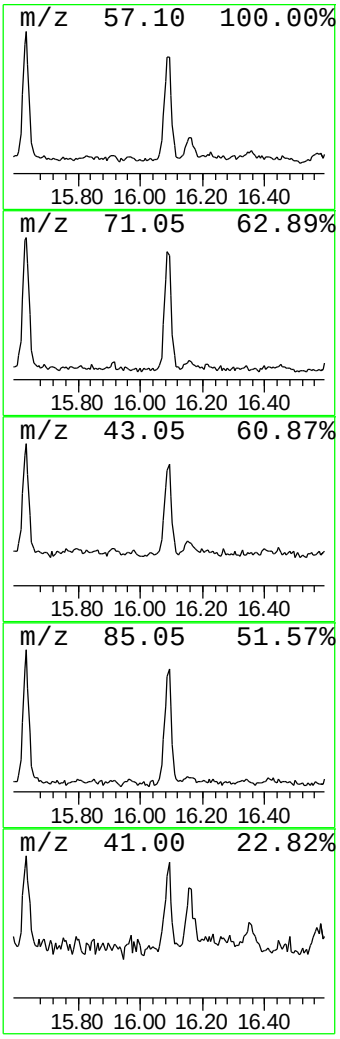
****

Peak Number 14 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.09	3.91 ng	123521	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heneicosane	296	C21H44	000629-94-7	90
5	Pentacosane	352	C25H52	000629-99-2	90





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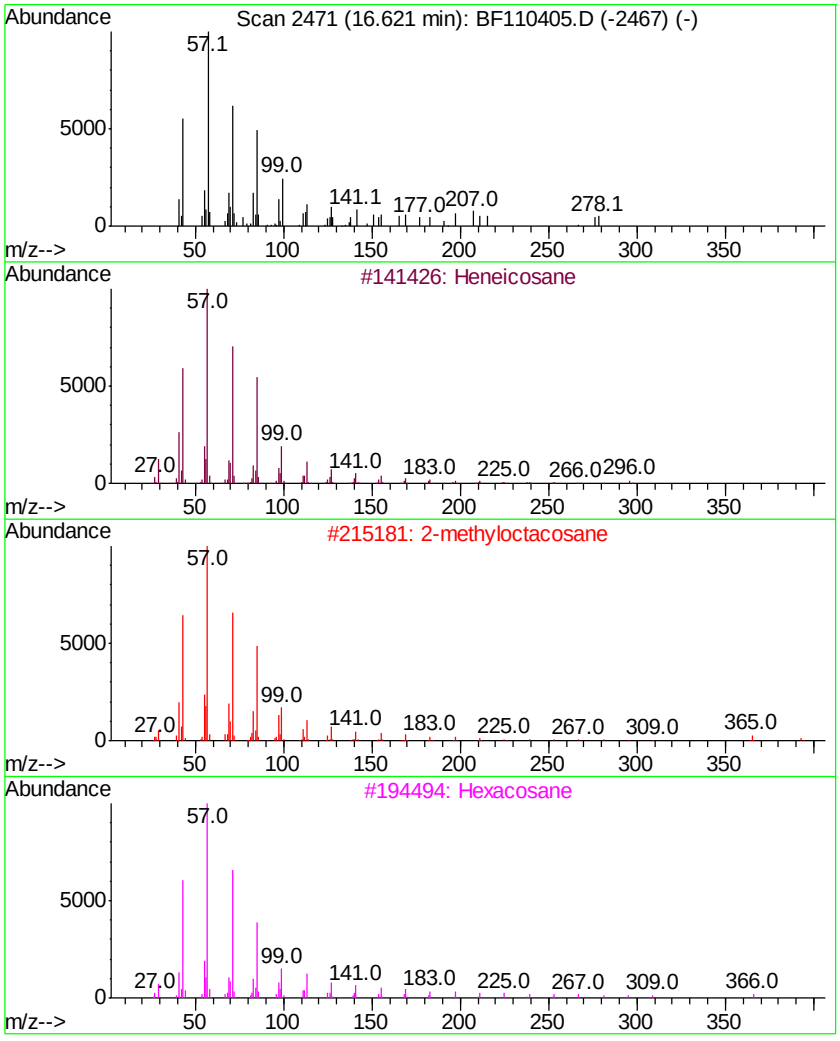
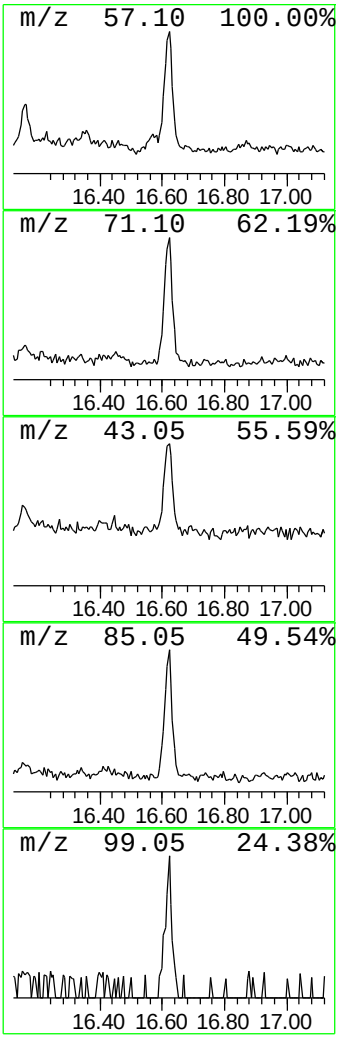
Peak Number 15 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.62	2.82 ng	89268	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	86
2	2-methyloctacosane	408	C29H60	1000376-72-8	83
3	Hexacosane	366	C26H54	000630-01-3	83
4	Tetratetracontane	619	C44H90	007098-22-8	80
5	Octacosane	394	C28H58	000630-02-4	80





Tentatively Identified Compound (LSC) summary

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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...	2.29	16.7	ng	390508	1	6.95	468637	20.0
2-Pentanone, 4-hy...	5.20	3.7	ng	86355	1	6.95	468637	20.0
unknown6.72	6.72	81.1	ng	1900980	1	6.95	468637	20.0
Benzene, 4-ethyl-...	8.45	2.0	ng	63675	2	8.24	628573	20.0
Benzene, 1-methyl...	8.51	2.4	ng	73781	2	8.24	628573	20.0
unknown11.83	11.83	2.4	ng	73325	4	11.49	618143	20.0
1,2-Benzenedicarb...	12.03	2.3	ng	69553	4	11.49	618143	20.0
11H-Benzo[a]fluorene	13.26	2.1	ng	53634	5	14.13	516856	20.0
Octacosyl trifluo...	13.95	7.4	ng	190152	5	14.13	516856	20.0
unknown14.26	14.26	4.3	ng	109910	5	14.13	516856	20.0
Octacosane	14.57	2.8	ng	72387	5	14.13	516856	20.0
Hexadecane	14.89	4.0	ng	102043	5	14.13	516856	20.0
Hexacosane	16.09	3.9	ng	123521	6	15.66	632116	20.0
Heneicosane	16.62	2.8	ng	89268	6	15.66	632116	20.0