LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012418\
Data File : BF102412.D
Acq On : 25 Jan 2018 1:28
Operator : SJ/JU
Sample : J1235-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 32-2

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:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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	3.693	266	273	278	rBV	40978	63535	2.14%	0.252%
2	4.916	475	481	492	rBV	174956	258887	8.73%	1.026%
3	5.328	546	551	564	rBV	2621556	2781176	93.73%	11.017%
4	6.363	721	727	743	rBV	2463156	2967116	100.00%	11.754%
5	6.487	743	748	751	rBV	3061695	2846809	95.95%	11.277%
6	6.710	783	786	795	rBV	798588	754467	25.43%	2.989%
7	6.869	809	813	816	rBV	2489366	2140486	72.14%	8.479%
8	7.281	878	883	886	rBV	1788169	1761265	59.36%	6.977%
9	7.998	1000	1005	1017	rBV	1024896	1005938	33.90%	3.985%
10	9.075	1183	1188	1191	rBV	2989812	2739365	92.32%	10.851%
11	9.469	1250	1255	1263	rBV	459778	410622	13.84%	1.627%
12	9.681	1287	1291	1295	rBV	74297	66229	2.23%	0.262%
13	9.751	1295	1303	1312	rVV	1048786	1070734	36.09%	4.242%
14	10.175	1372	1375	1379	rVB	88066	72997	2.46%	0.289%
15	10.404	1406	1414	1419	rBV3	88430	120909	4.07%	0.479%
16	10.539	1433	1437	1445	rBV	1506709	1375207	46.35%	5.448%
17	10.604	1445	1448	1453	rVV	85423	111150	3.75%	0.440%
18	10.651	1453	1456	1462	rVB	71039	79294	2.67%	0.314%
19	11.233	1551	1555	1558	rBV	1012476	864617	29.14%	3.425%
20	11.792	1647	1650	1654	rBV	117153	101179	3.41%	0.401%
21	12.816	1820	1824	1828	rBV	1946676	1898128	63.97%	7.519%
22	13.710	1973	1976	1987	rVB	216197	249318	8.40%	0.988%
23	13.869	1999	2003	2010	rVB	702241	654899	22.07%	2.594%
24	14.345	2080	2084	2088	rBV2	54631	72019	2.43%	0.285%
25	14.951	2184	2187	2190	rBV	40404	48639	1.64%	0.193%
26	15.298	2241	2246	2254	rVB	502345	655505	22.09%	2.597%
27	15.721	2314	2318	2323	rVB2	49823	73694	2.48%	0.292%

Sum of corrected areas: 25244184

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Misc :
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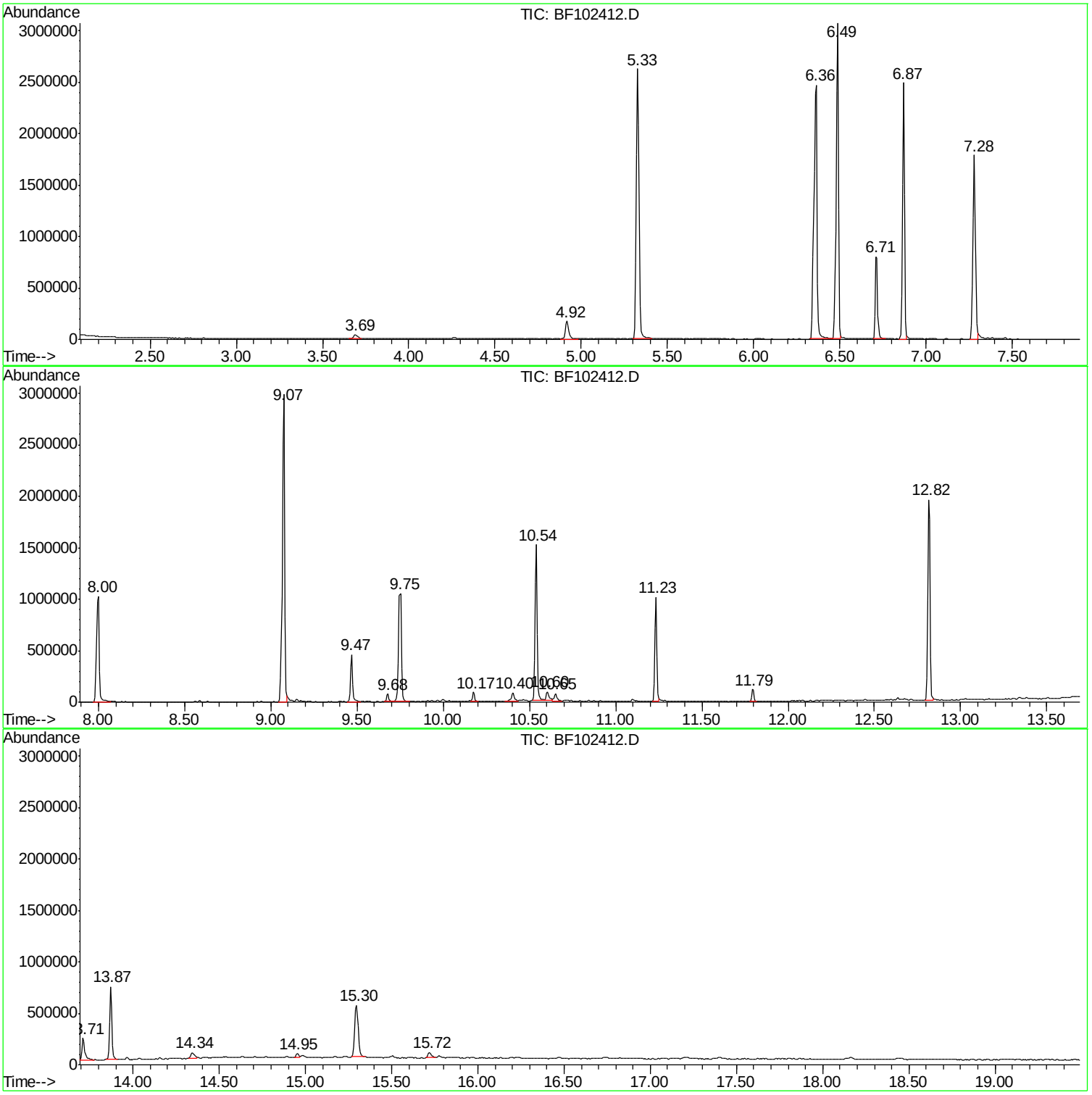
Instrument : BNA_F
ClientSampleId : 32-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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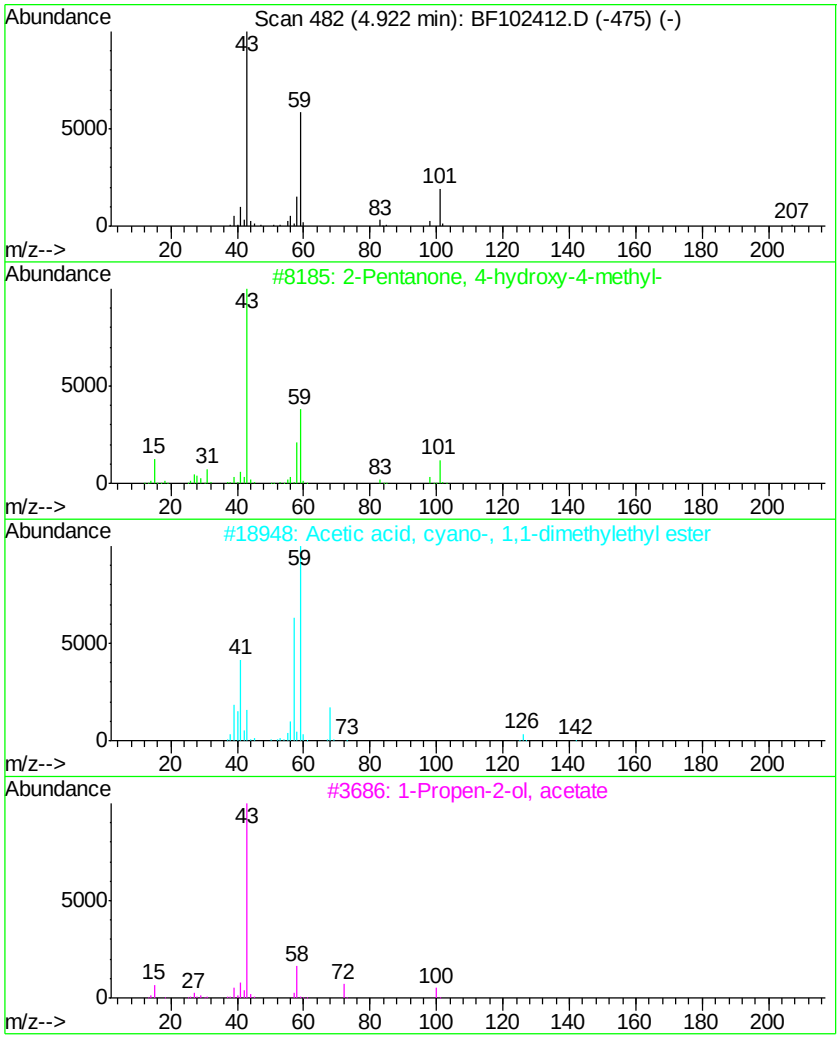
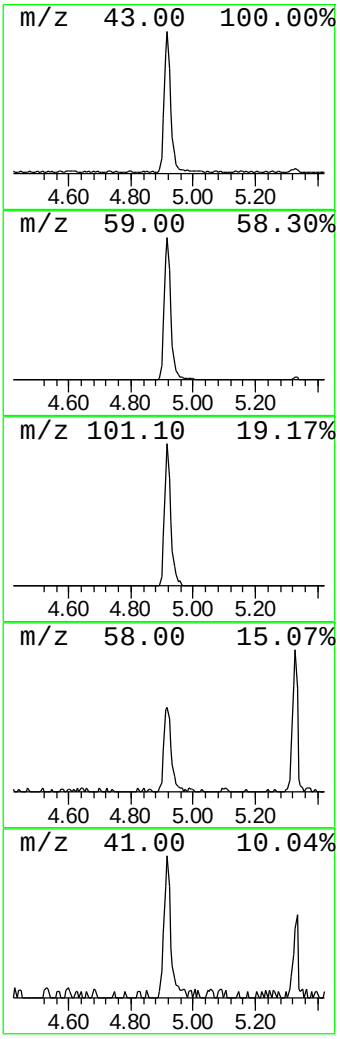
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	6.86 ng	258887	1,4-Dichlorobenzene-d4	6.72

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	1,2-Butanediol	90	C4H10O2	000584-03-2	9





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Sample : J1235-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 32-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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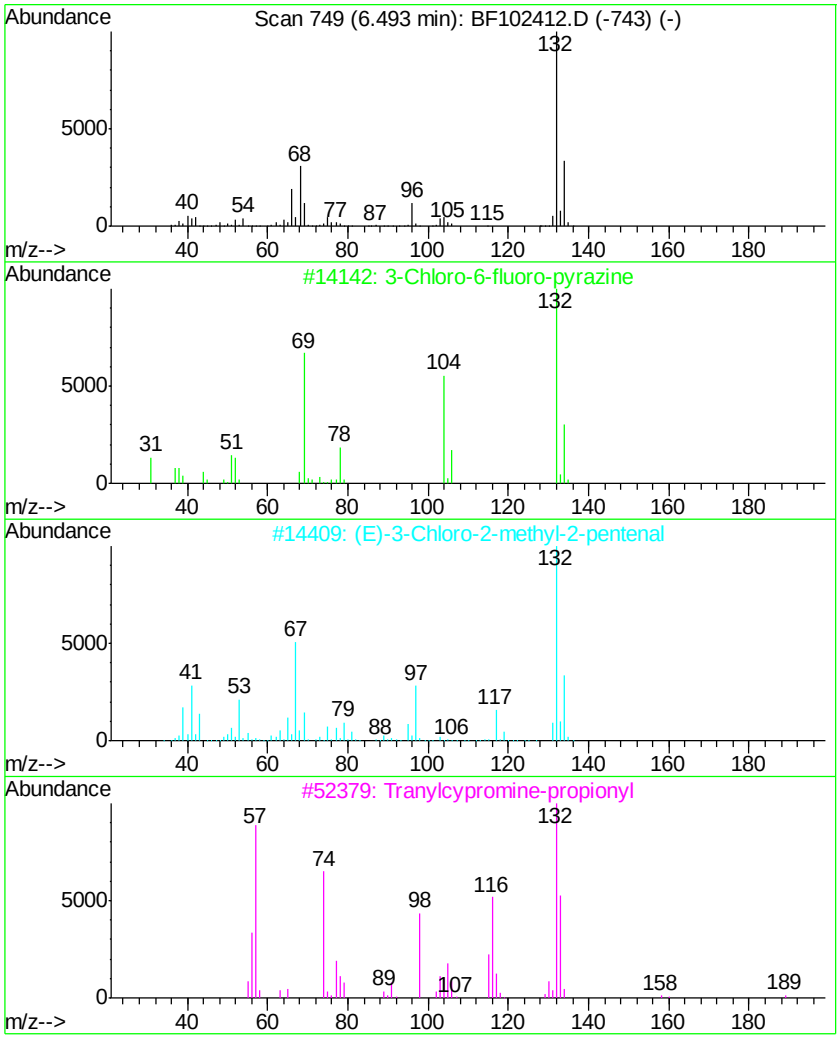
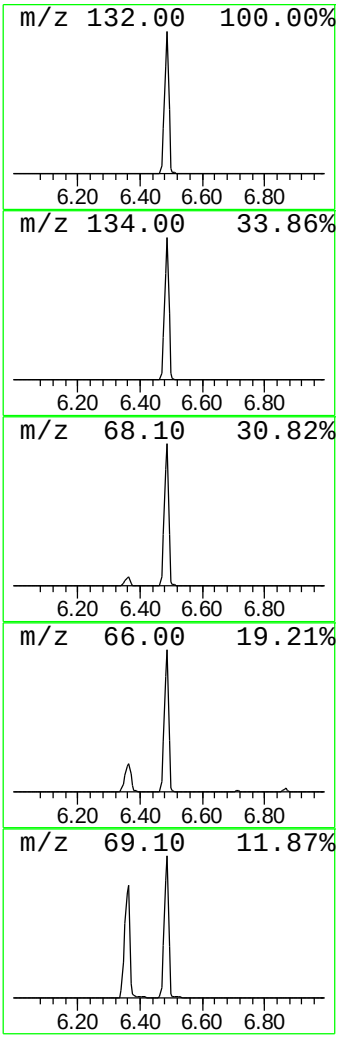
Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	75.47 ng	2846810	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 32-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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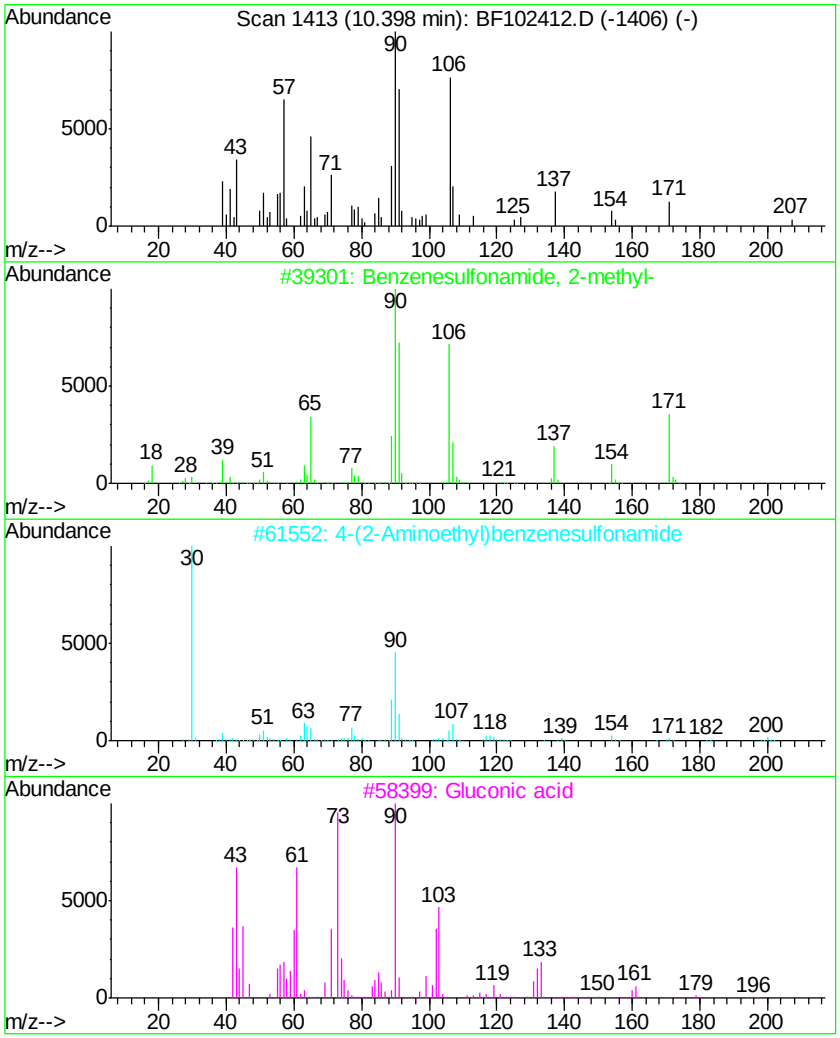
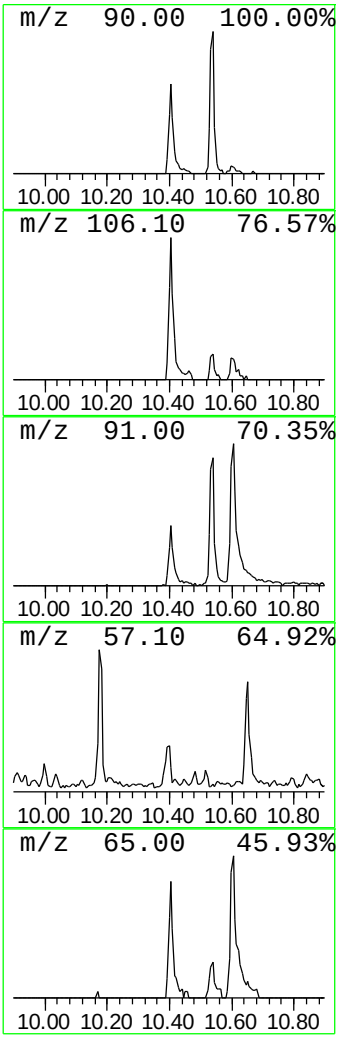
Peak Number 4 Benzenesulfonamide, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.40	2.26 ng	120909	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 2-methyl-	171	C7H9NO2S	000088-19-7	95
2	4-(2-Aminoethyl)benzenesulfonamide	200	C8H12N2O2S	035303-76-5	43
3	Gluconic acid	196	C6H12O7	000526-95-4	38
4	Thiourea, methyl-	90	C2H6N2S	000598-52-7	32
5	Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	32





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Sample : J1235-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 32-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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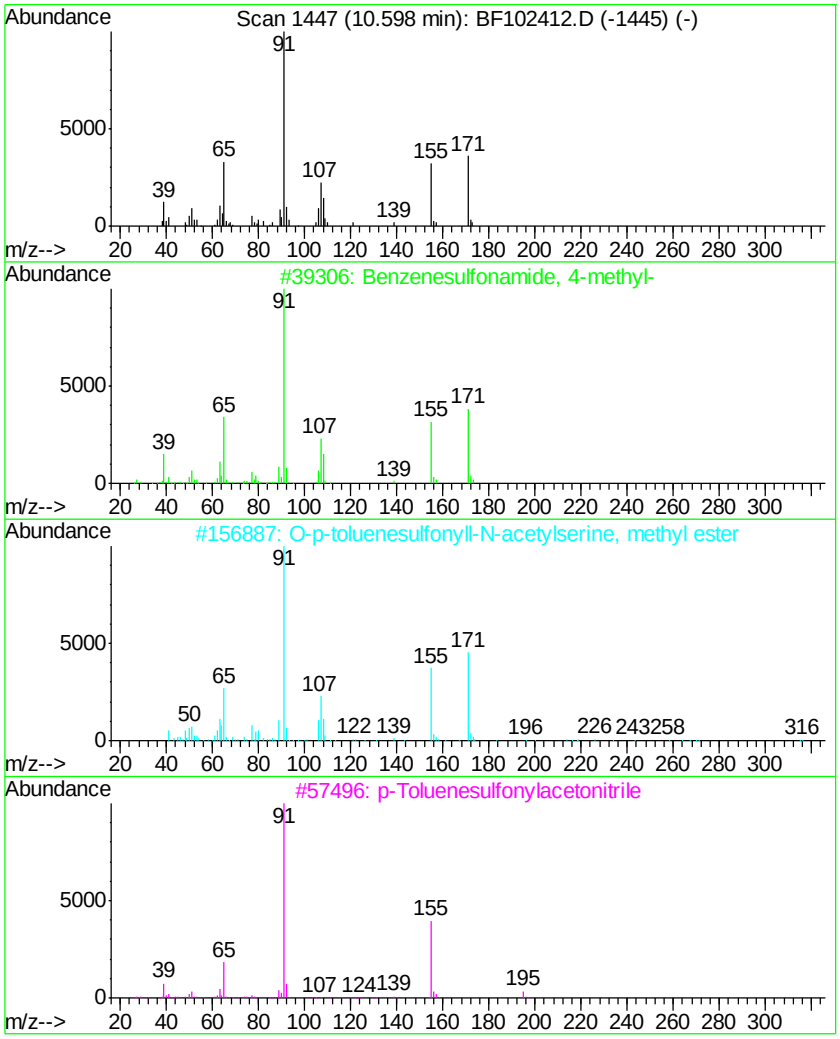
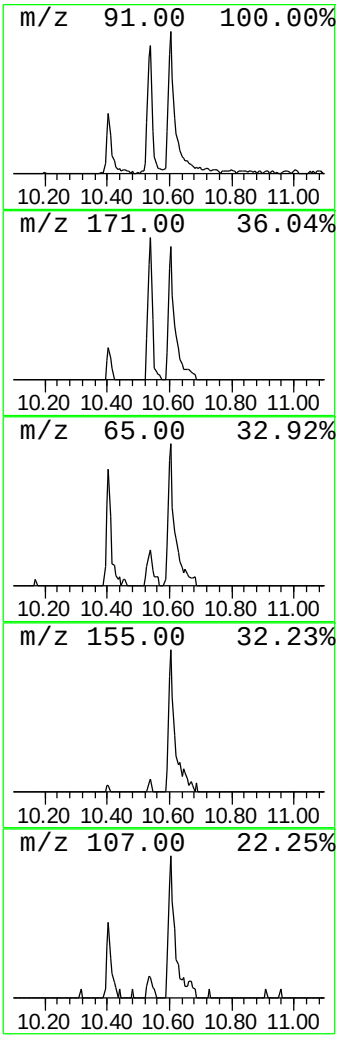
Peak Number 5 Benzenesulfonamide, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	2.57 ng	111150	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	96
2	O-p-toluenesulfonyll-N-acetylser...	315	C13H17NO6S	1000126-44-8	78
3	p-Toluenesulfonylacetonitrile	195	C9H9NO2S	005697-44-9	38
4	(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	38
5	4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	38





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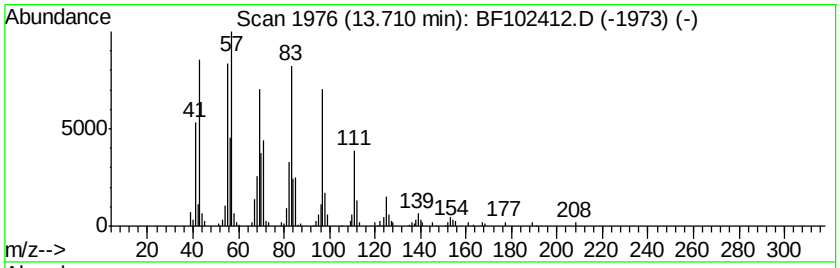
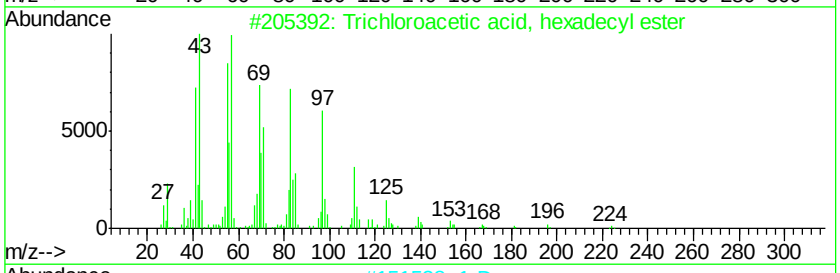
****

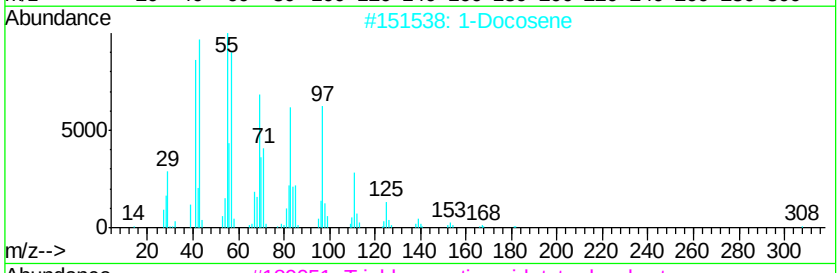
Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 3

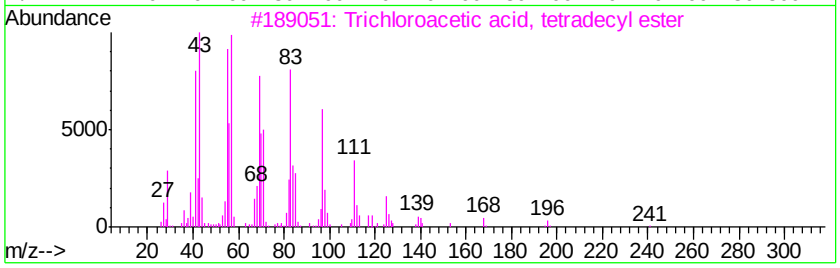
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	7.61 ng	249318	Chrysene-d12	13.87

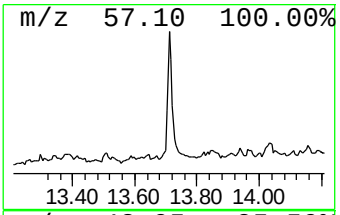
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	1-Docosene	308	C22H44	001599-67-3	91
3	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
5	1-Nonadecene	266	C19H38	018435-45-5	91

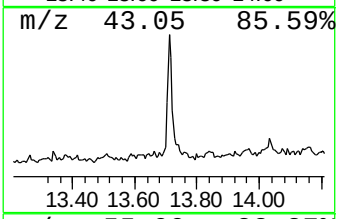


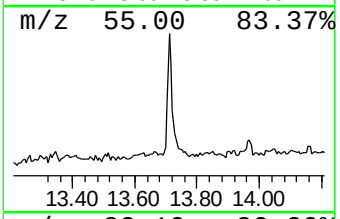


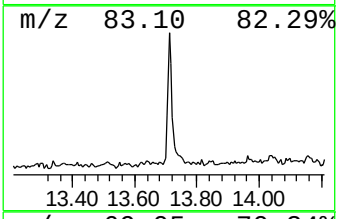


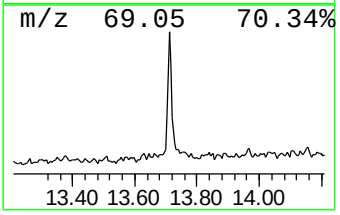












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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

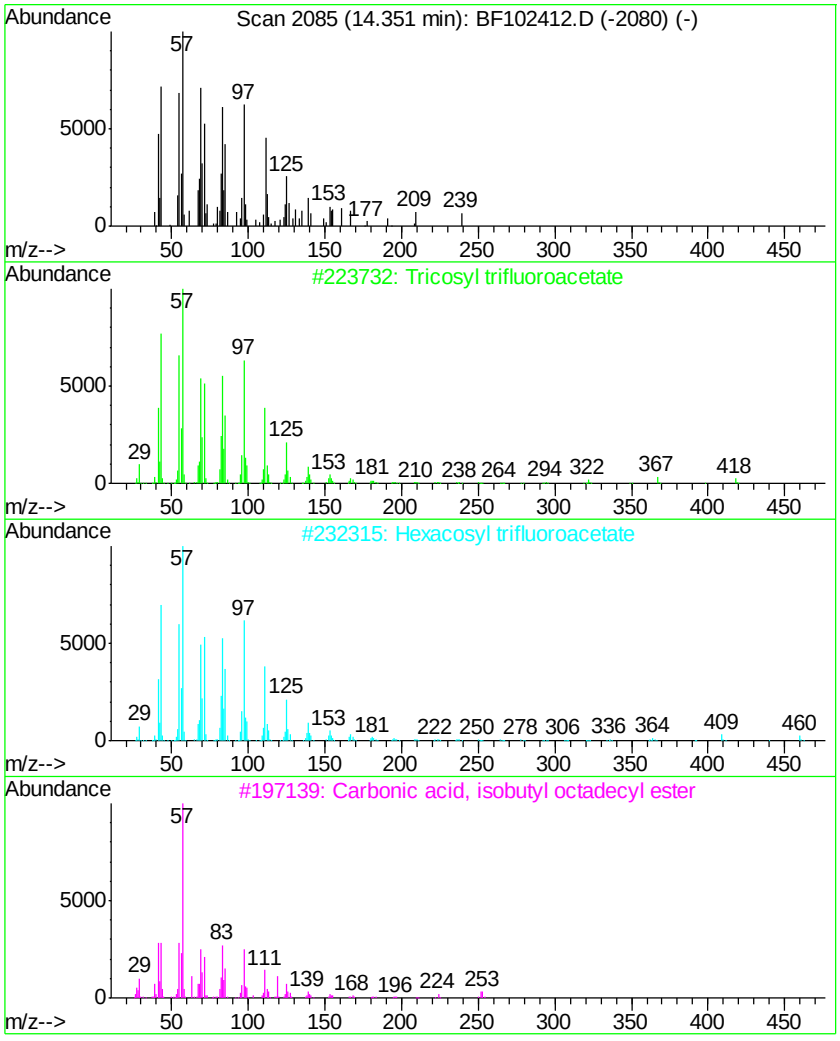
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

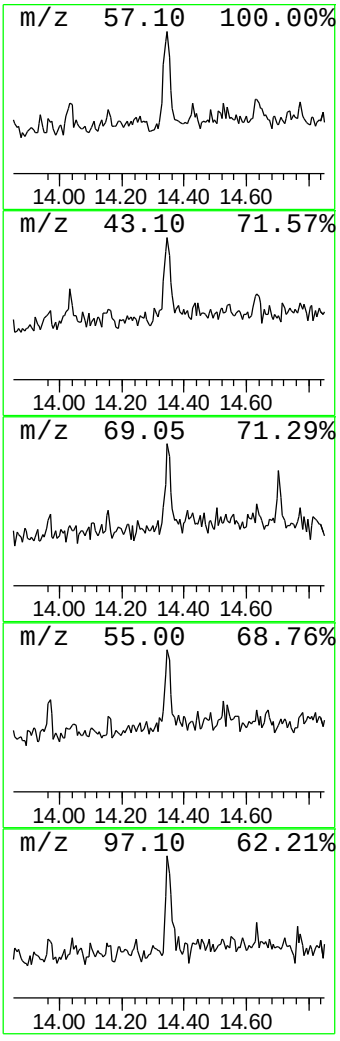
****

Peak Number 7 Tricosyl trifluoroacetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	2.20 ng	72019	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
2	Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	90
3	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	87
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	87
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87





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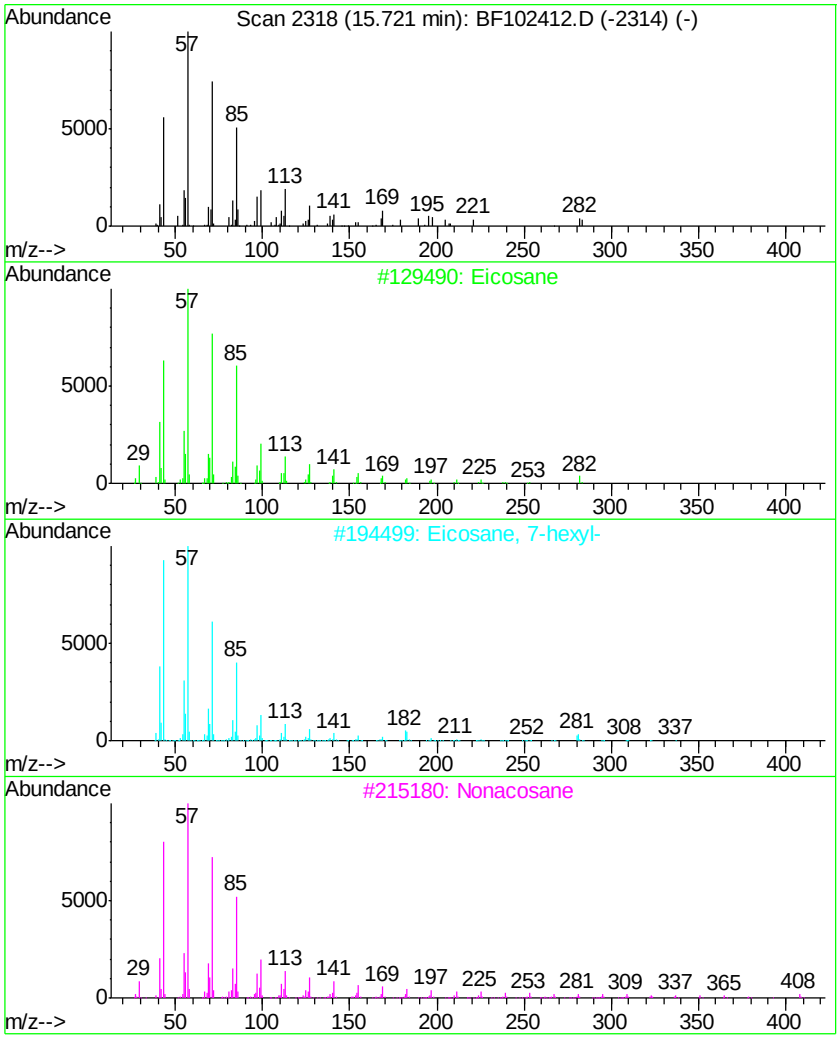
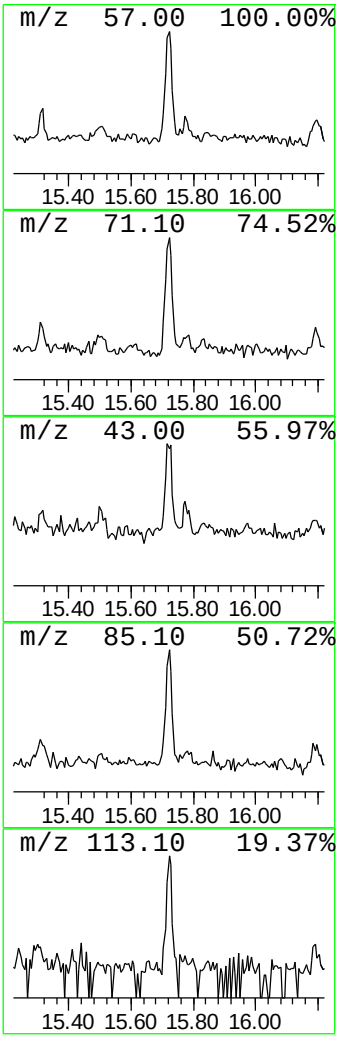
Peak Number 8 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	2.25 ng	73694	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	83
3	Nonacosane	408	C29H60	000630-03-5	83
4	Hexacosane	366	C26H54	000630-01-3	80
5	2-methyloctacosane	408	C29H60	1000376-72-8	80





Tentatively Identified Compound (LSC) summary

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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...	4.92	6.9	ng	258887	1	6.72	754467	20.0
unknown6.49	6.49	75.5	ng	2846810	1	6.72	754467	20.0
Benzenesulfonamid...	10.40	2.3	ng	120909	3	9.75	1070730	20.0
Benzenesulfonamid...	10.60	2.6	ng	111150	4	11.23	864617	20.0
Trichloroacetic a...	13.71	7.6	ng	249318	5	13.87	654899	20.0
Tricosyl trifluor...	14.35	2.2	ng	72019	5	13.87	654899	20.0
Eicosane	15.72	2.3	ng	73694	6	15.30	655505	20.0