LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080116\
Data File : BF089529.D
Acq On : 2 Aug 2016 00:26
Operator : UM/SJ
Sample : H4287-19
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-63-6.5-7.5

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:\HPCHEM1\BNA_F\METHODS\8270-BF072716.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	1.655	4	6	50	rVB	698151	1764890	100.00%	19.273%
2	4.559	257	260	272	rBV	134482	218505	12.38%	2.386%
3	5.050	301	303	329	rBV	622118	801592	45.42%	8.753%
4	6.147	396	399	406	rBV	570370	820160	46.47%	8.956%
5	6.250	406	408	410	rBV	729698	820008	46.46%	8.955%
6	6.479	426	428	435	rBV	177297	185863	10.53%	2.030%
7	6.627	439	441	444	rBV	466509	618611	35.05%	6.755%
8	7.050	476	478	489	rBV	413693	494555	28.02%	5.401%
9	7.199	489	491	497	rVB	16104	24669	1.40%	0.269%
10	7.770	538	541	543	rBV	160755	224604	12.73%	2.453%
11	8.845	633	635	637	rBV	981465	850724	48.20%	9.290%
12	9.245	668	670	673	rBV	280152	232976	13.20%	2.544%
13	9.508	691	693	695	rBV	272476	237804	13.47%	2.597%
14	10.296	760	762	764	rBV	285114	377804	21.41%	4.126%
15	10.433	772	774	777	rBV	22889	26102	1.48%	0.285%
16	10.982	819	822	824	rBV	152880	183898	10.42%	2.008%
17	11.542	869	871	876	rBB	12854	21588	1.22%	0.236%
18	12.456	948	951	957	rVB	21868	38804	2.20%	0.424%
19	12.559	957	960	963	rBV	673598	616541	34.93%	6.733%
20	12.811	978	982	986	rBV	25958	40681	2.31%	0.444%
21	13.005	996	999	1001	rBV	18940	23918	1.36%	0.261%
22	13.474	1037	1040	1045	rBV	54819	74222	4.21%	0.811%
23	13.599	1048	1051	1056	rBV	187847	217102	12.30%	2.371%
24	14.925	1165	1167	1173	rBV	198781	223801	12.68%	2.444%
25	15.611	1225	1227	1231	rBV2	11455	18047	1.02%	0.197%

Sum of corrected areas: 9157469

LSC Report - Integrated Chromatogram

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Operator : UM/SJ
Sample : H4287-19
Misc :
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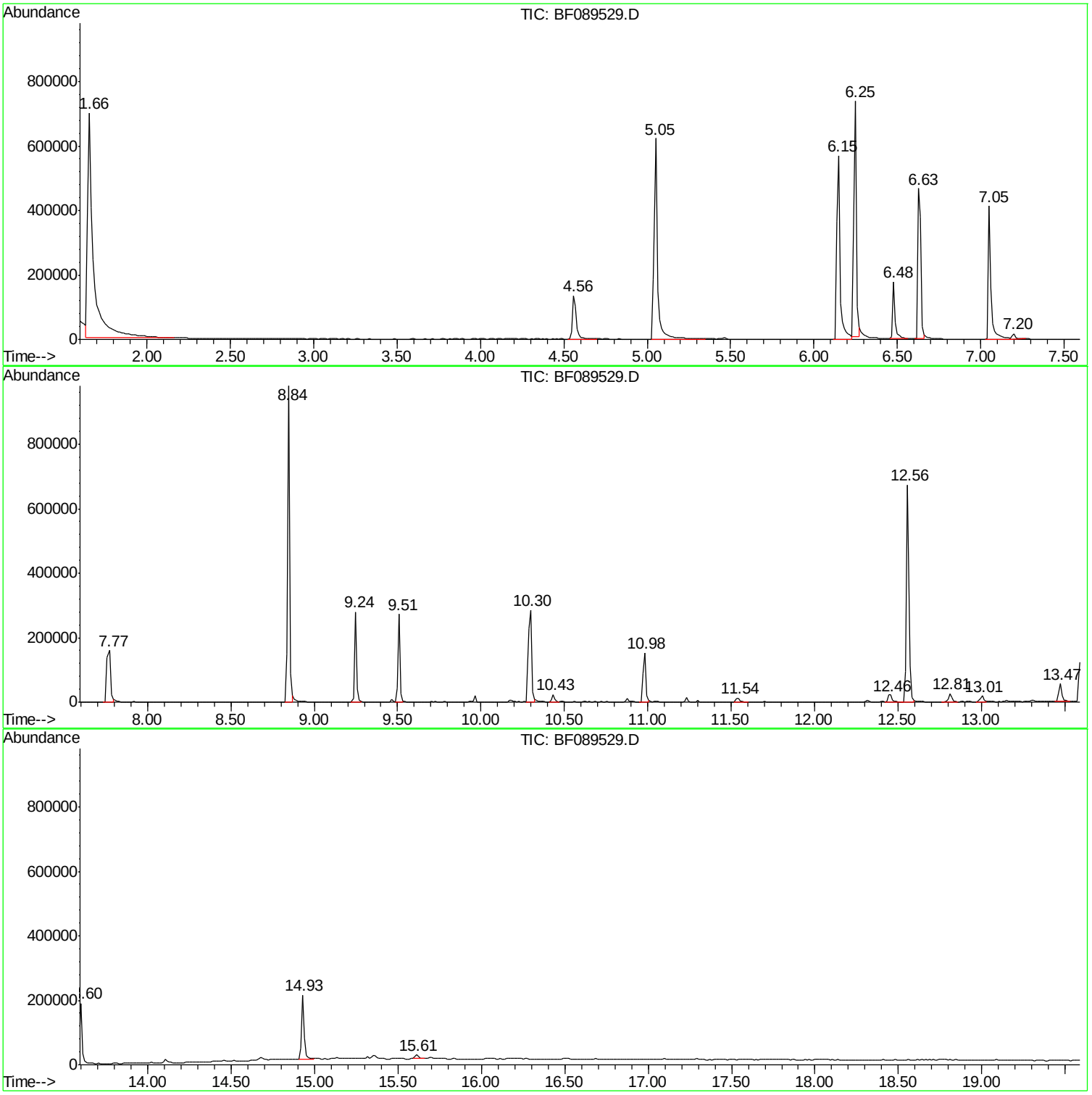
Instrument : BNA_F
ClientSampleId : SB-63-6.5-7.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.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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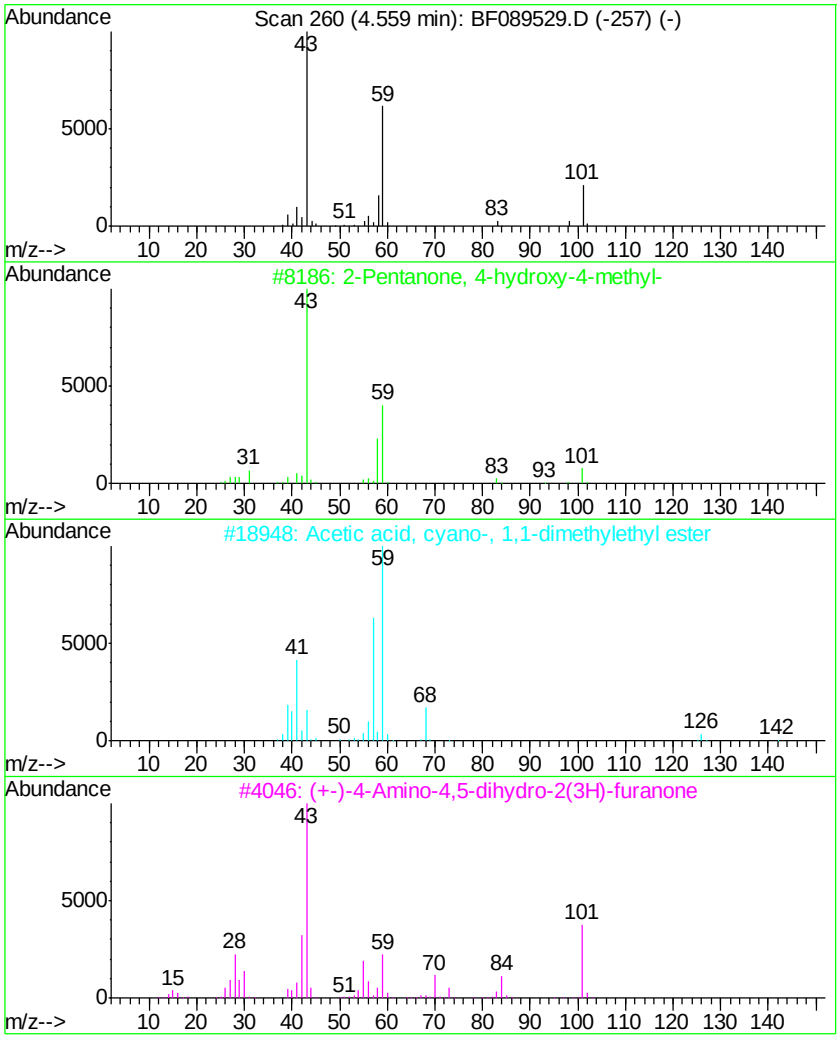
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

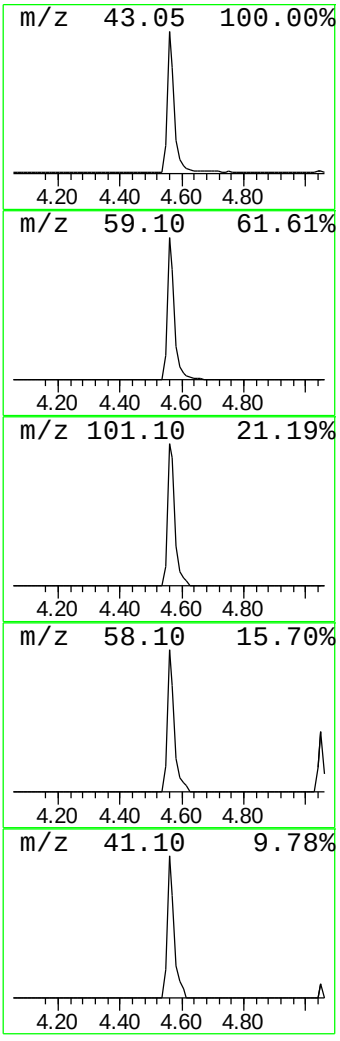
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.56	23.51 ng	218505	1,4-Dichlorobenzene-d4	6.48

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Operator : UM/SJ
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Instrument : BNA_F
ClientSampleId : SB-63-6.5-7.5

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TIC Library : C:\Database\NIST11.L
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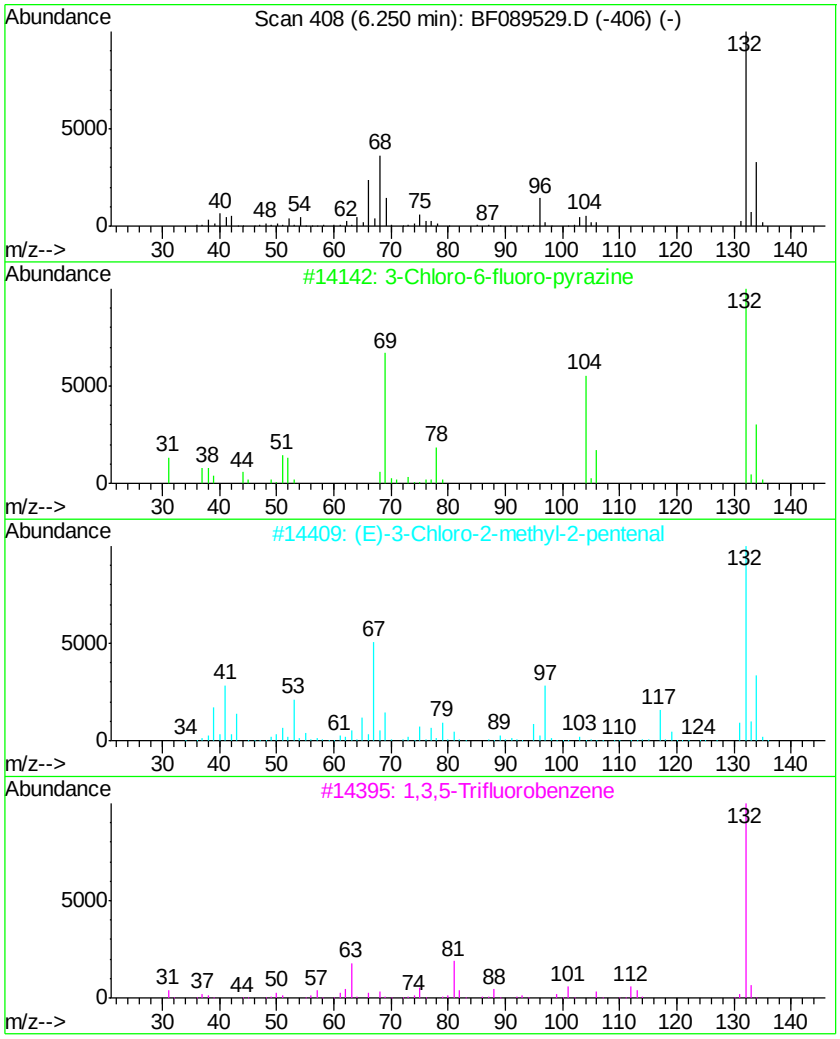
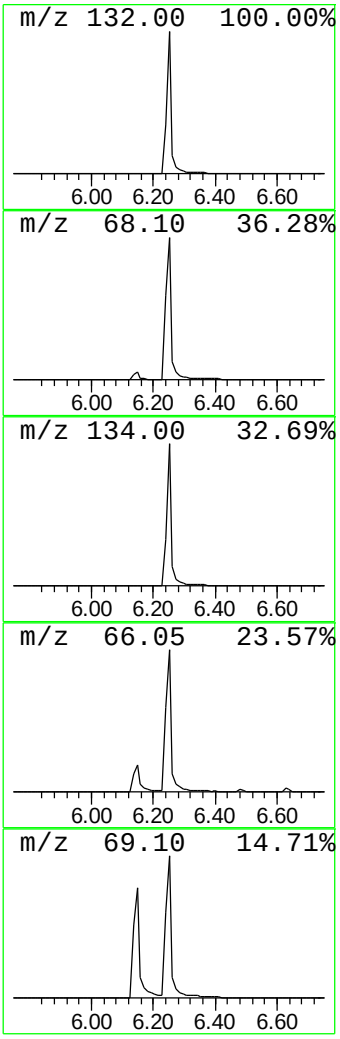
****

Peak Number 3 unknown6.25 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.25	88.24 ng	820008	1,4-Dichlorobenzene-d4	6.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Operator : UM/SJ
Sample : H4287-19
Misc :
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Instrument : BNA_F
ClientSampleId : SB-63-6.5-7.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
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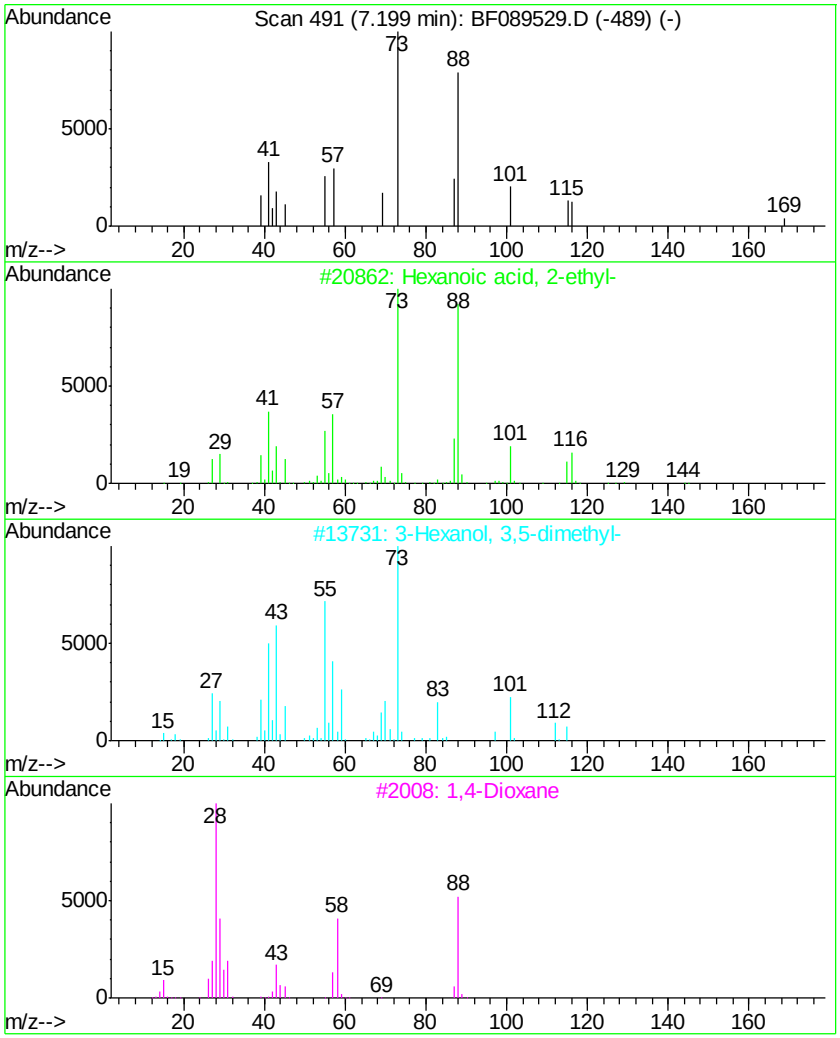
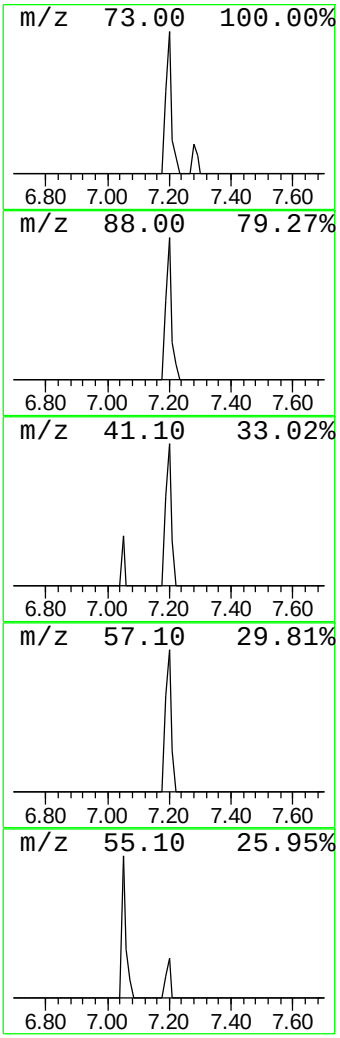
****

Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	2.20 ng	24669	Naphthalene-d8	7.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	72
2	3-Hexanol, 3,5-dimethyl-	130	C8H18O	004209-91-0	10
3	1,4-Dioxane	88	C4H8O2	000123-91-1	9
4	1-Methyl-1-silacyclopentan-1-ol	116	C5H12OSi	1000216-84-4	9
5	.alpha.-D-Mannofuranoside, 1-O-d...	320	C16H32O6	1000160-04-7	9





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ClientSampleId : SB-63-6.5-7.5

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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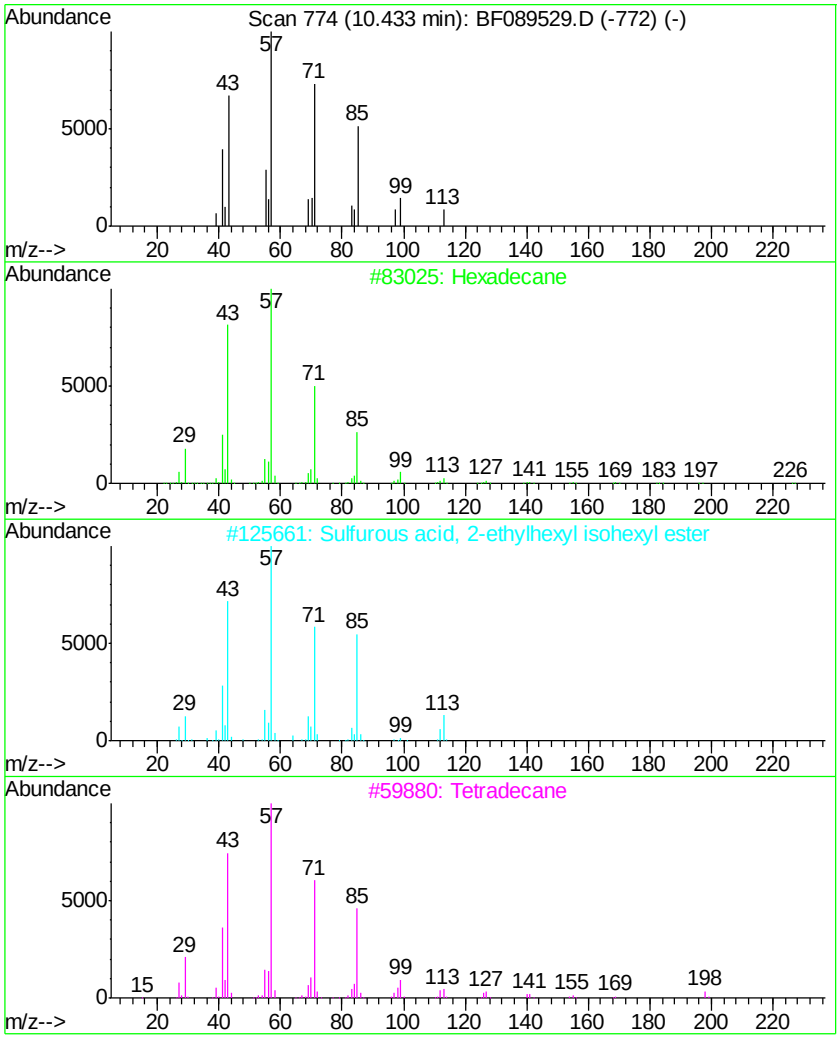
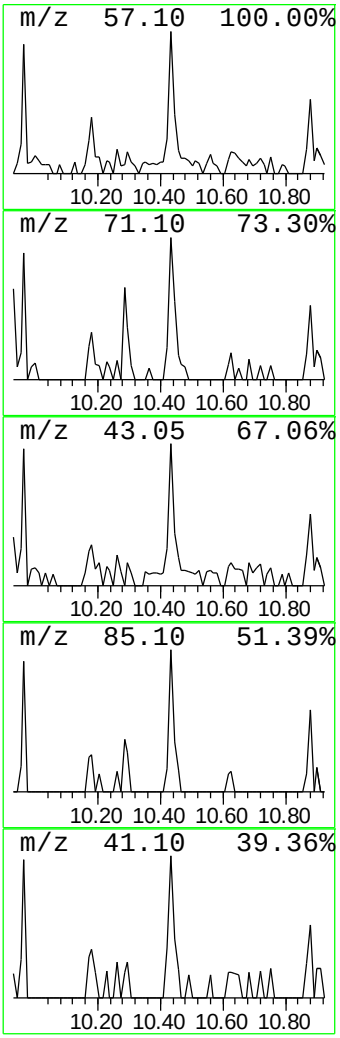
****

Peak Number 6 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.43	2.84 ng	26102	Phenanthrene-d10	10.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	83
2	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	78
3	Tetradecane	198	C14H30	000629-59-4	72
4	Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	64
5	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	64





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Instrument : BNA_F
ClientSampleId : SB-63-6.5-7.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
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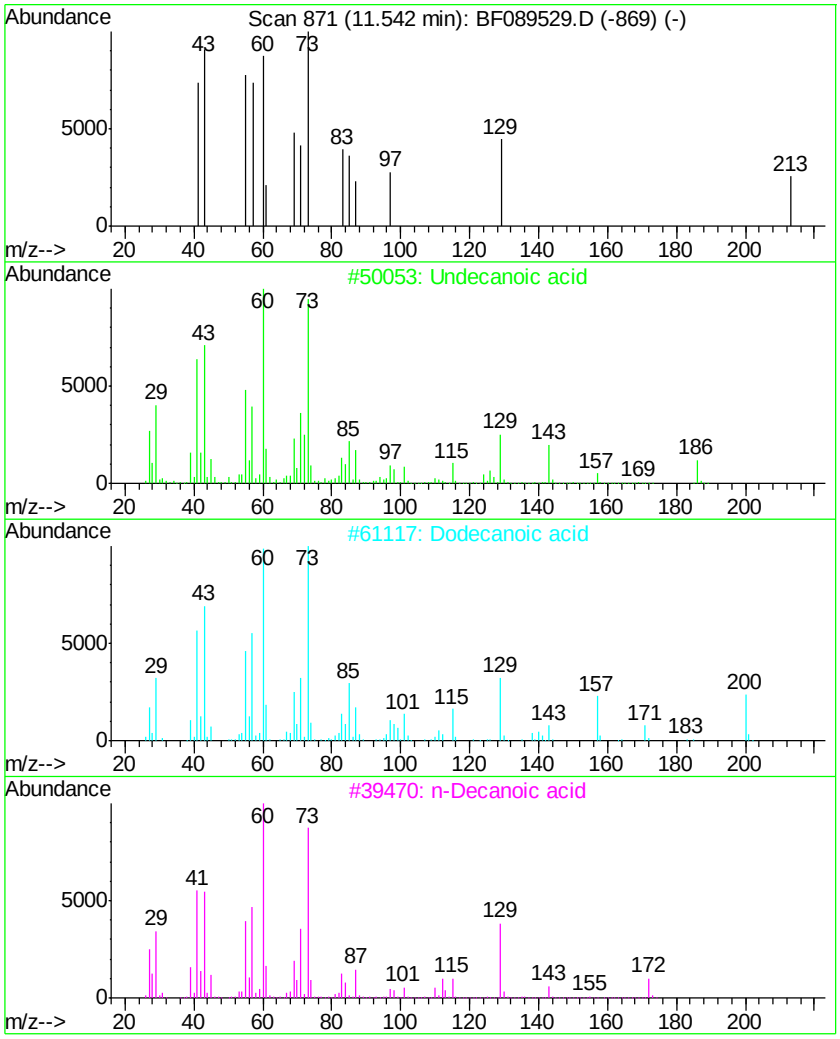
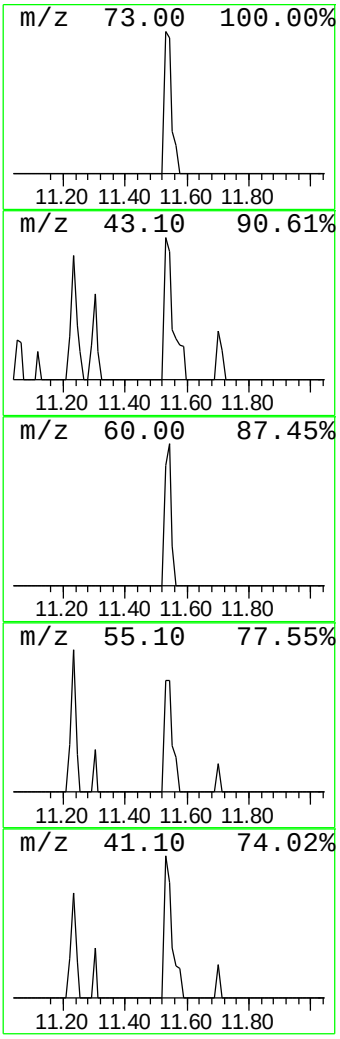
****

Peak Number 7 Undecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.54	2.35 ng	21588	Phenanthrene-d10	10.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	53
2	Dodecanoic acid	200	C12H24O2	000143-07-7	53
3	n-Decanoic acid	172	C10H20O2	000334-48-5	50
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	40
5	Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	22





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Instrument : BNA_F
ClientSampleId : SB-63-6.5-7.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

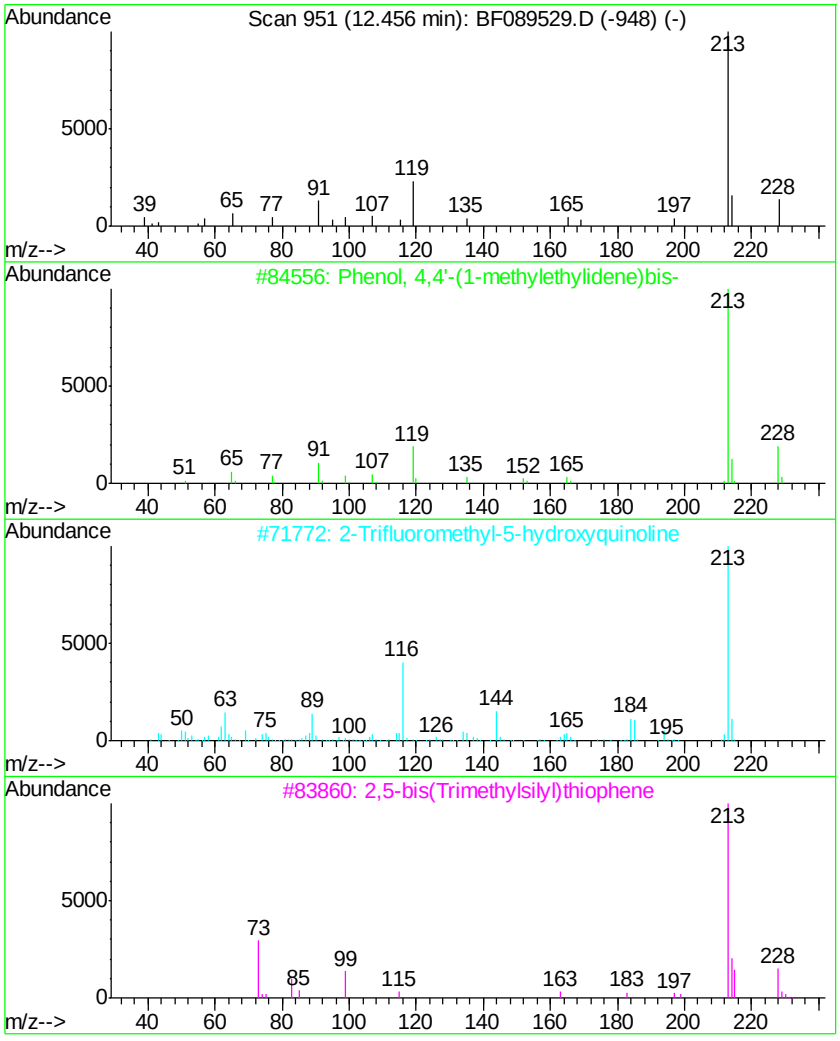
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

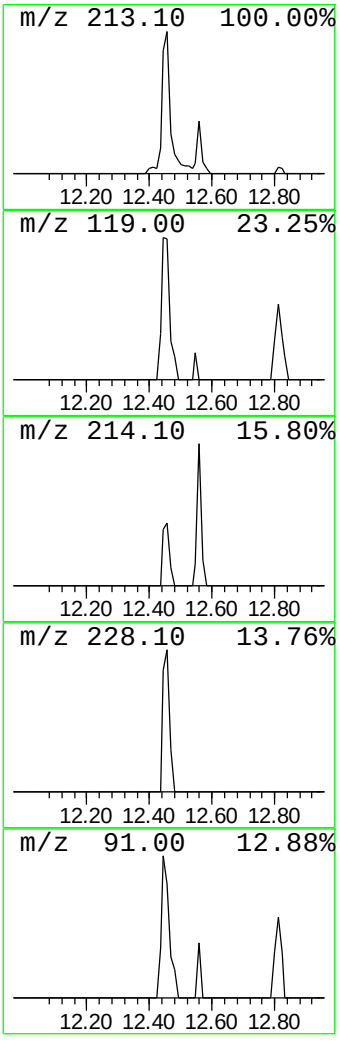
****

Peak Number 8 Phenol, 4,4'-(1-methylethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.46	3.57 ng	38804	Chrysene-d12	13.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	86
2	2-Trifluoromethyl-5-hydroxyquino...	213	C10H6F3NO	041958-06-9	50
3	2,5-bis(Trimethylsilyl)thiophene	228	C10H20SSi2	017906-71-7	50
4	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	47
5	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	40





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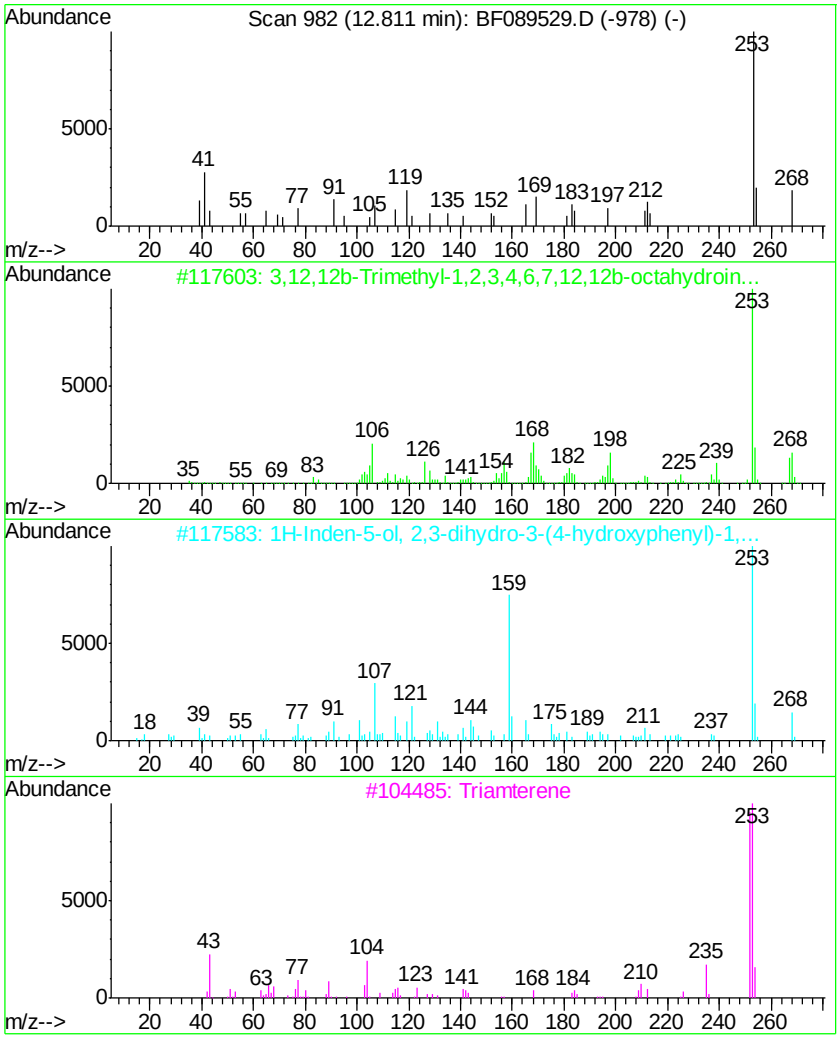
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

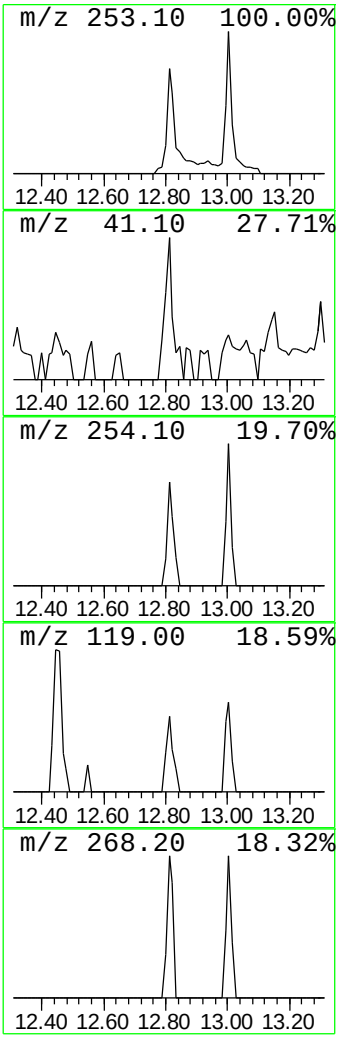
****

Peak Number 9 3,12,12b-Trimethyl-1,2,3,4,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.81	3.75 ng	40681	Chrysene-d12	13.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,12,12b-Trimethyl-1,2,3,4,6,7,1...	268	C18H24N2	082605-35-4	59
2	1H-Inden-5-ol, 2,3-dihydro-3-(4-...	268	C18H20O2	010527-11-4	50
3	Triamterene	253	C12H11N7	000396-01-0	47
4	Indolo[2,3-a]quinolizin-4(12H)-o...	268	C17H20N2O	020156-09-6	42
5	Phenol, 4-(3,4-dihydro-2,2,4-tri...	268	C18H20O2	000472-41-3	38





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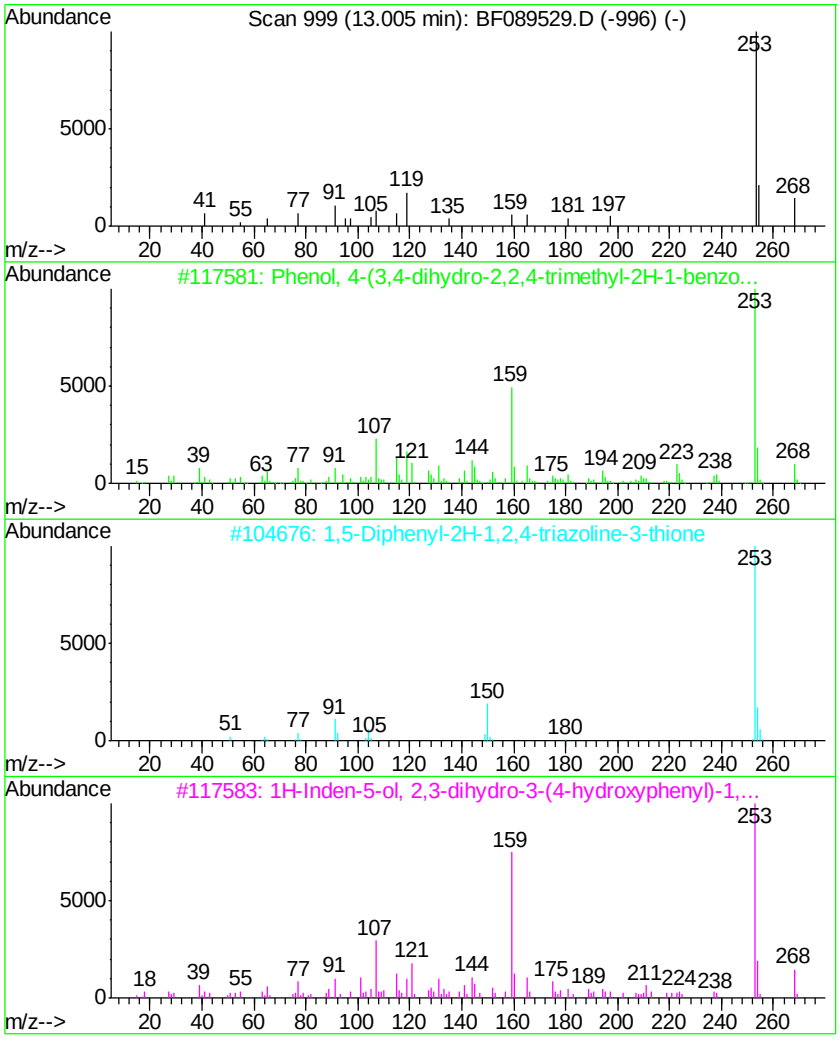
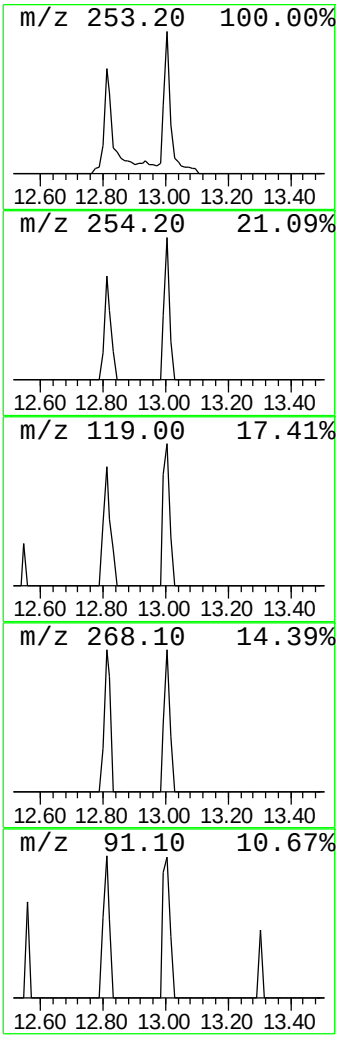
****

Peak Number 10 Phenol, 4-(3,4-dihydro-2,2,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.01	2.20 ng	23918	Chrysene-d12	13.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(3,4-dihydro-2,2,4-tri...	268	C18H20O2	000472-41-3	50
2	1,5-Diphenyl-2H-1,2,4-triazoline...	253	C14H11N3S	005055-74-3	40
3	1H-Inden-5-ol, 2,3-dihydro-3-(4-...	268	C18H20O2	010527-11-4	9
4	2-Chloro-11H-pyrido[3',2'-4,5]py...	253	C14H8ClN3	1000212-59-3	9
5	3-Chloro-11H-pyrido[3',2'-4,5]py...	253	C14H8ClN3	1000212-59-4	9





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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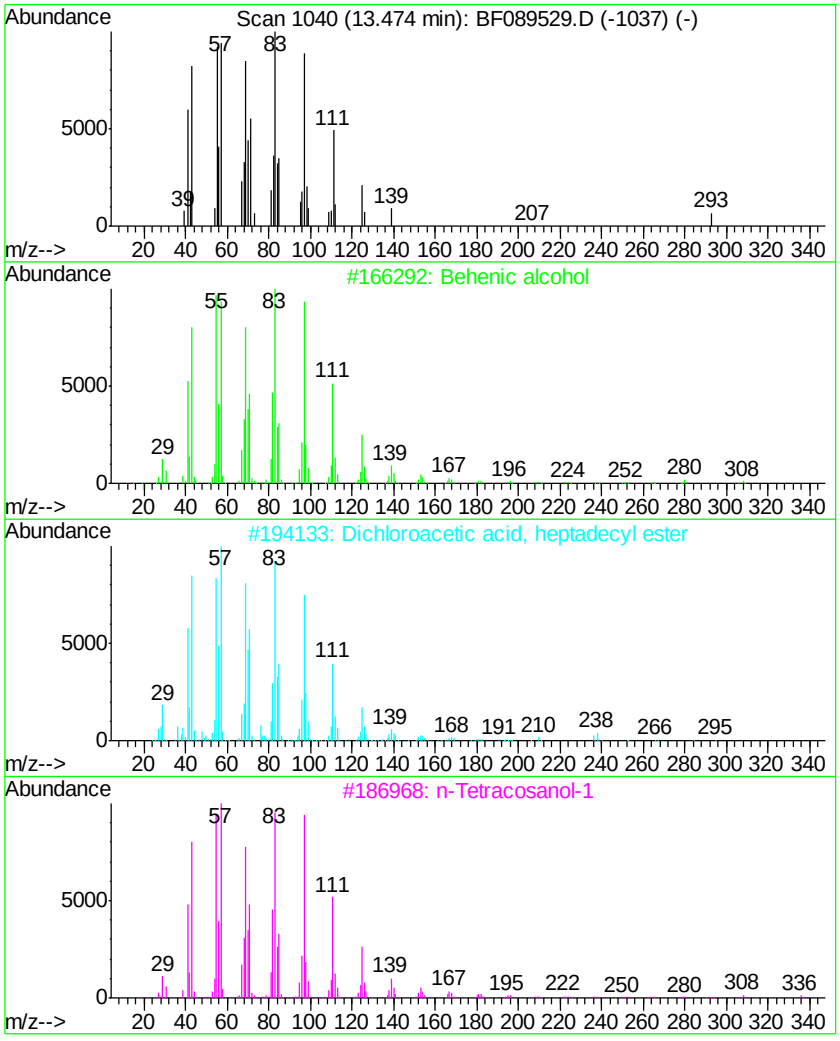
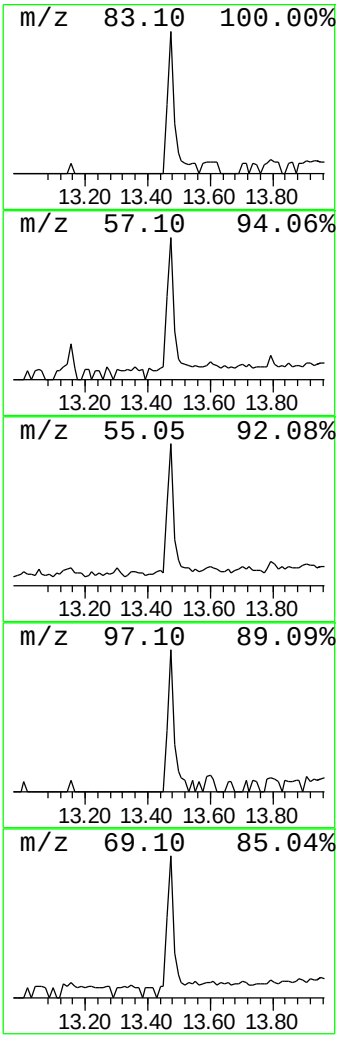
****

Peak Number 11 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	6.84 ng	74222	Chrysene-d12	13.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.56	23.5	ng	218505	1	6.48	185863	20.0
unknown6.25	6.25	88.2	ng	820008	1	6.48	185863	20.0
Hexanoic acid, 2-...	7.20	2.2	ng	24669	2	7.77	224604	20.0
Hexadecane	10.43	2.8	ng	26102	4	10.98	183898	20.0
Undecanoic acid	11.54	2.4	ng	21588	4	10.98	183898	20.0
Phenol, 4,4'-(1-m...	12.46	3.6	ng	38804	5	13.60	217102	20.0
3,12,12b-Trimethy...	12.81	3.8	ng	40681	5	13.60	217102	20.0
Phenol, 4-(3,4-di...	13.01	2.2	ng	23918	5	13.60	217102	20.0
Behenic alcohol	13.47	6.8	ng	74222	5	13.60	217102	20.0