

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050417\
 Data File : BF094890.D
 Acq On : 4 May 2017 23:51
 Operator : SJ/MA
 Sample : I2930-04
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-1-COMP

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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	5.037	522	527	542	rBV	268899	530074	18.57%	1.985%
2	5.672	630	635	662	rBV	1743325	2605383	91.29%	9.758%
3	6.243	728	732	740	rVB	21479	32584	1.14%	0.122%
4	7.272	901	907	921	rBV	1846647	2709785	94.95%	10.149%
5	7.384	921	926	938	rVB	2128499	2853989	100.00%	10.689%
6	7.719	979	983	993	rVB	438290	527438	18.48%	1.975%
7	7.960	1019	1024	1036	rVB	1767663	2053725	71.96%	7.692%
8	8.619	1130	1136	1145	rBV	1259561	1687382	59.12%	6.320%
9	8.948	1184	1192	1198	rBV3	14053	29867	1.05%	0.112%
10	9.736	1322	1326	1339	rBV	553916	698179	24.46%	2.615%
11	11.519	1623	1629	1639	rBV	2310658	2798733	98.06%	10.482%
12	12.201	1740	1745	1753	rBV	643736	797040	27.93%	2.985%
13	12.566	1803	1807	1816	rBV2	599704	795804	27.88%	2.981%
14	13.413	1947	1951	1958	rVB2	34726	43612	1.53%	0.163%
15	13.866	2022	2028	2042	rBV	1368751	1863357	65.29%	6.979%
16	14.189	2079	2083	2085	rBV2	41534	55070	1.93%	0.206%
17	14.213	2085	2087	2091	rVB	37463	38774	1.36%	0.145%
18	14.613	2150	2155	2159	rBV4	17695	32275	1.13%	0.121%
19	14.918	2203	2207	2211	rBV	32723	37943	1.33%	0.142%
20	14.971	2211	2216	2220	rVV	639301	834115	29.23%	3.124%
21	15.007	2220	2222	2228	rVB	34358	43523	1.52%	0.163%
22	15.942	2377	2381	2390	rVB	215509	272296	9.54%	1.020%
23	16.171	2416	2420	2425	rBV2	19148	29680	1.04%	0.111%
24	16.554	2479	2485	2489	rBV9	13552	29256	1.03%	0.110%
25	16.754	2515	2519	2522	rBV	62687	74676	2.62%	0.280%
26	17.024	2562	2565	2567	rBV	103498	110531	3.87%	0.414%
27	17.054	2567	2570	2576	rVB	94275	117940	4.13%	0.442%
28	17.301	2606	2612	2615	rBV	2212200	2704637	94.77%	10.130%
29	18.548	2819	2824	2832	rBV2	78621	161068	5.64%	0.603%
30	18.630	2834	2838	2843	rVV	596459	765191	26.81%	2.866%
31	18.701	2847	2850	2855	rVB	66443	70691	2.48%	0.265%
32	19.336	2954	2958	2965	rVB3	38888	69802	2.45%	0.261%
33	19.901	3050	3054	3057	rBV	39502	61795	2.17%	0.231%
34	20.053	3076	3080	3083	rBV	87465	101911	3.57%	0.382%

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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-BF050217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	20.083	3083	3085	3091	rVB5	27490	45148	1.58%	0.169%
36	20.189	3100	3103	3108	rBV	29555	38922	1.36%	0.146%
37	20.242	3109	3112	3116	rVV	42935	52770	1.85%	0.198%
38	20.295	3117	3121	3132	rVB	481900	599237	21.00%	2.244%
39	20.430	3141	3144	3148	rBV2	24747	32641	1.14%	0.122%
40	20.830	3208	3212	3221	rBV8	28874	77896	2.73%	0.292%
41	21.095	3254	3257	3262	rVB6	29616	41674	1.46%	0.156%
42	21.606	3340	3344	3351	rVB4	34779	63642	2.23%	0.238%
43	23.747	3699	3708	3715	rBV8	37116	109521	3.84%	0.410%

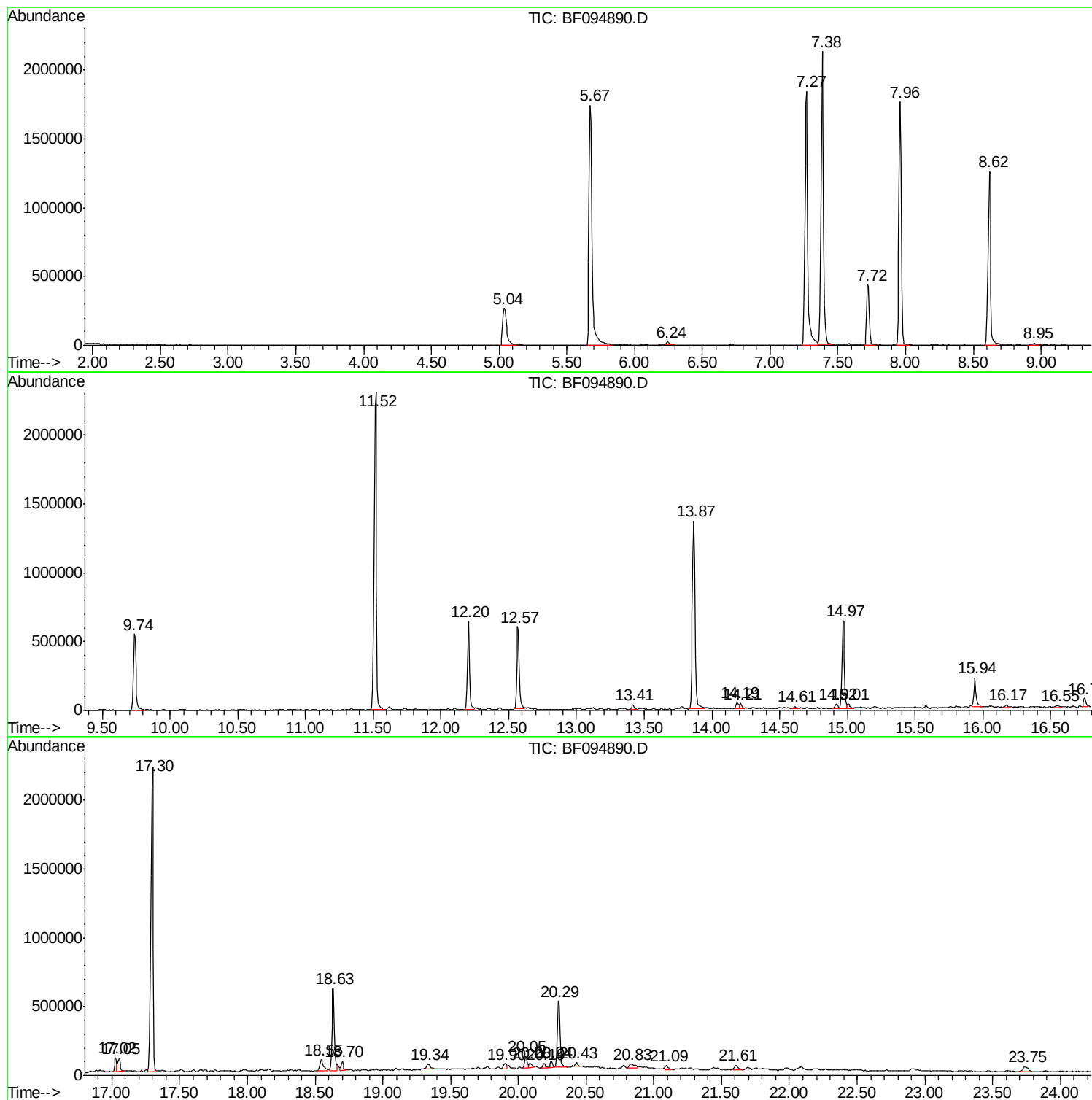
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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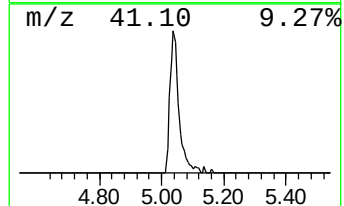
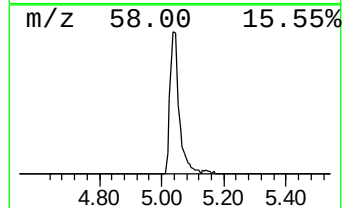
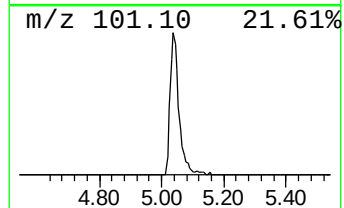
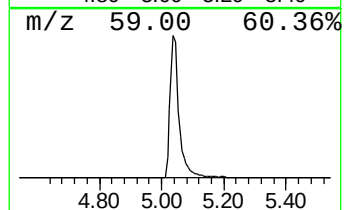
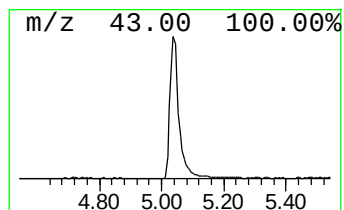
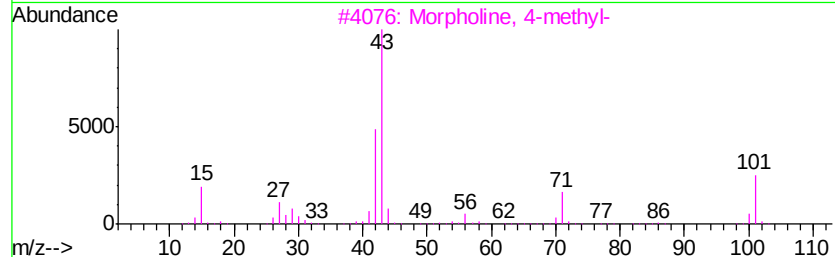
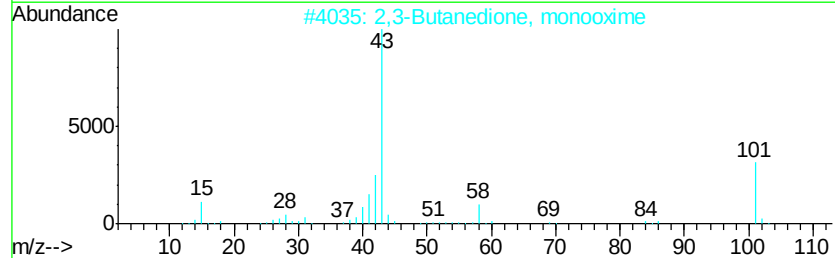
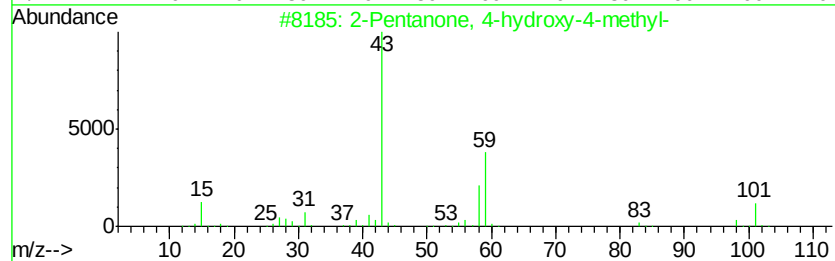
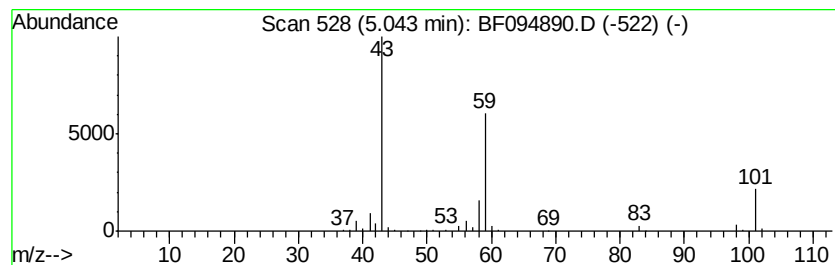
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.04	20.10 ng	530074	1,4-Dichlorobenzene-d4	7.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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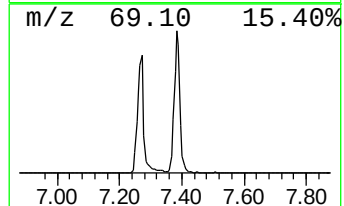
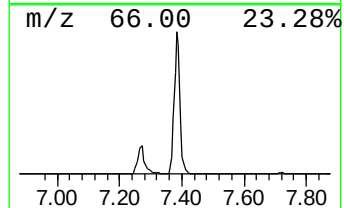
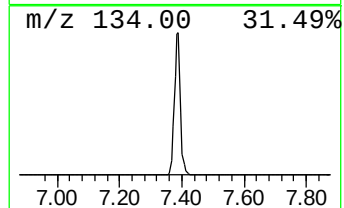
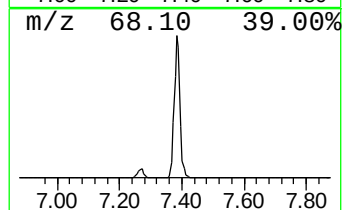
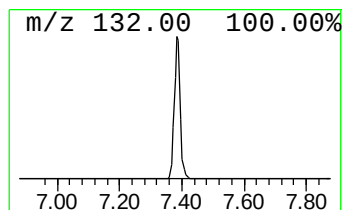
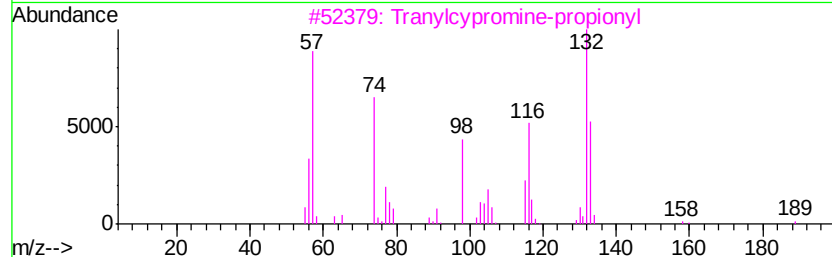
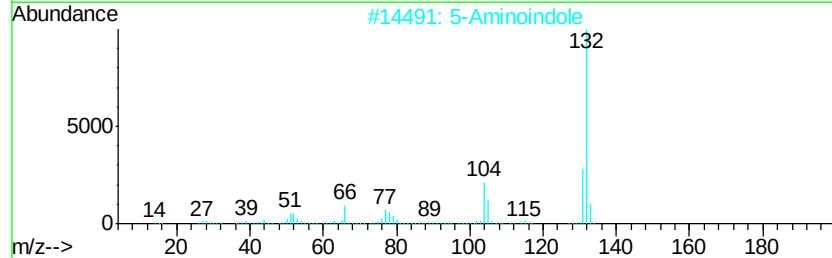
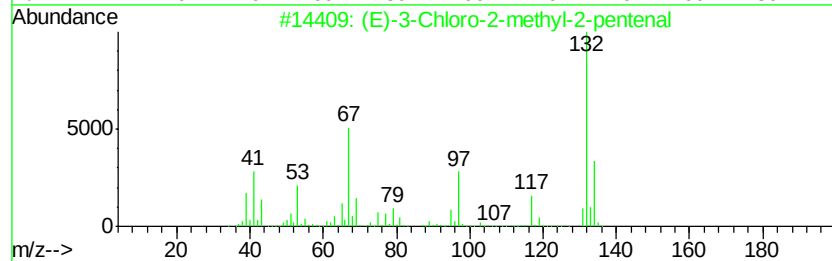
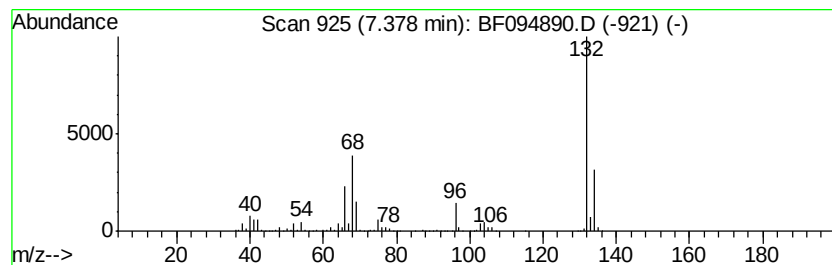
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Peak Number 2 unknown7.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	108.22 ng	2853990	1,4-Dichlorobenzene-d4	7.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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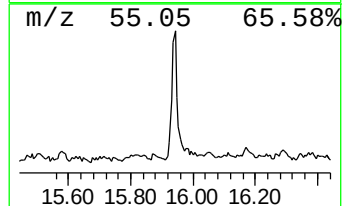
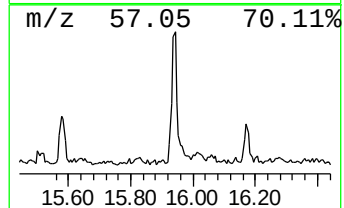
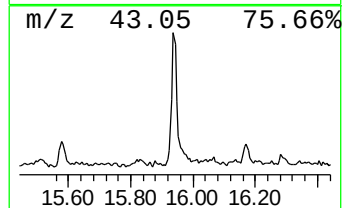
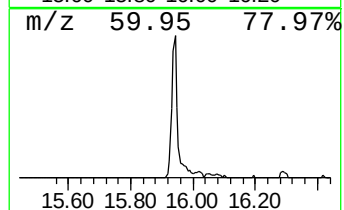
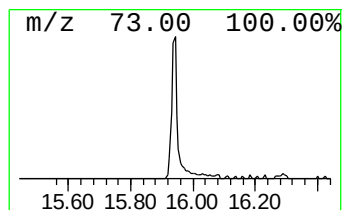
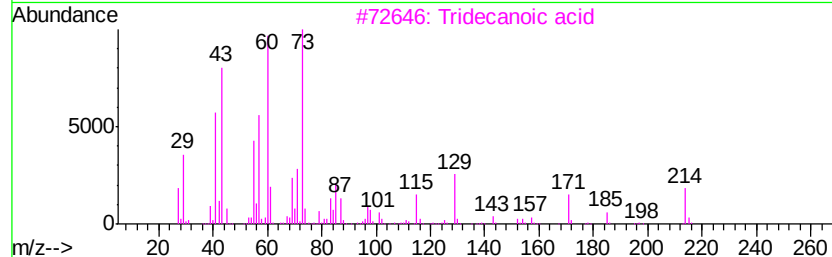
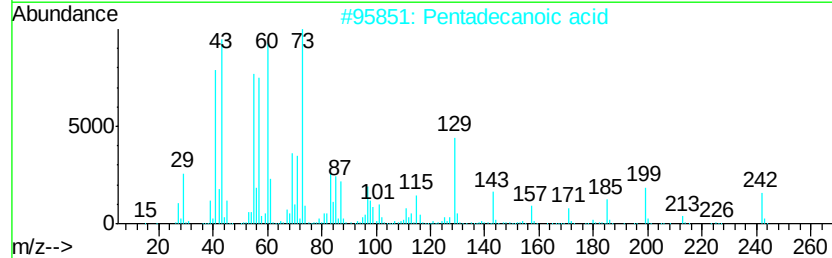
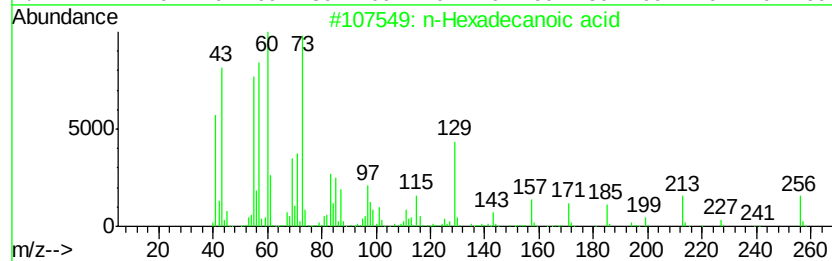
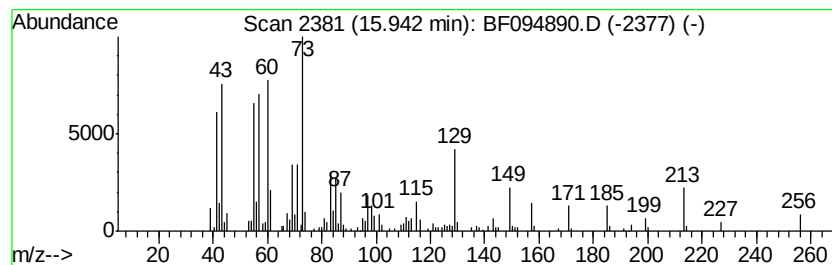
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.94	6.53 ng	272296	Phenanthrene-d10	14.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58



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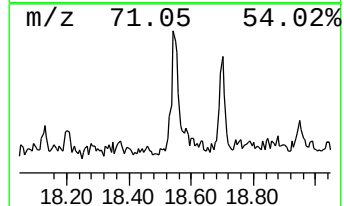
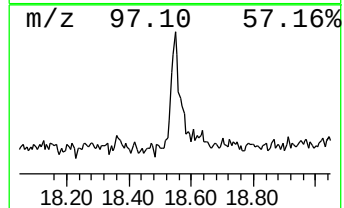
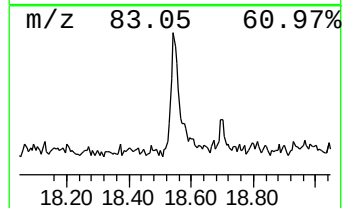
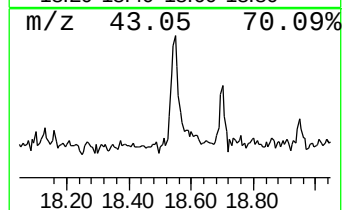
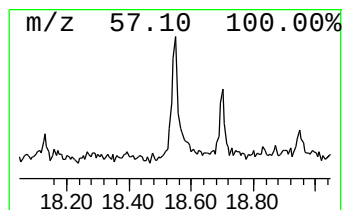
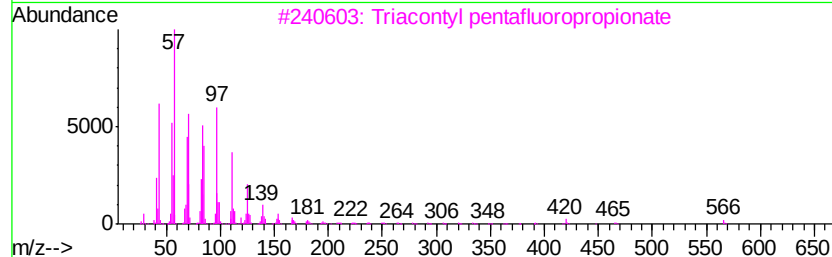
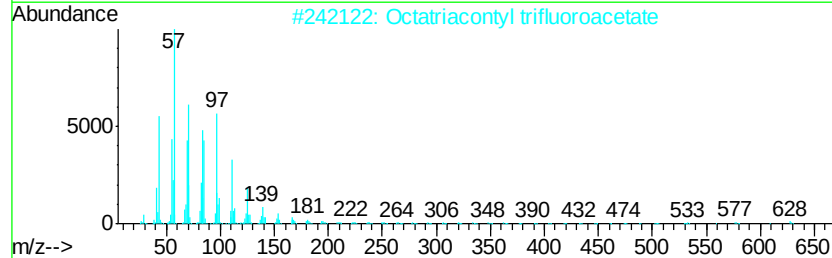
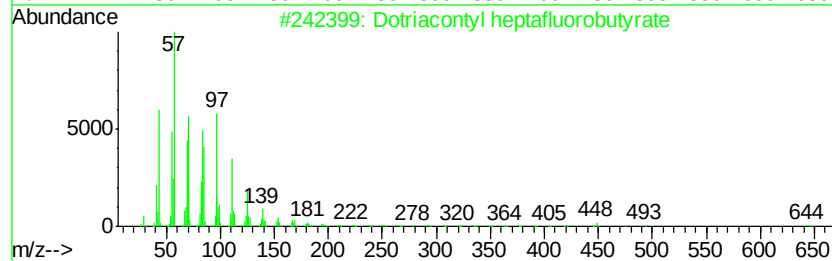
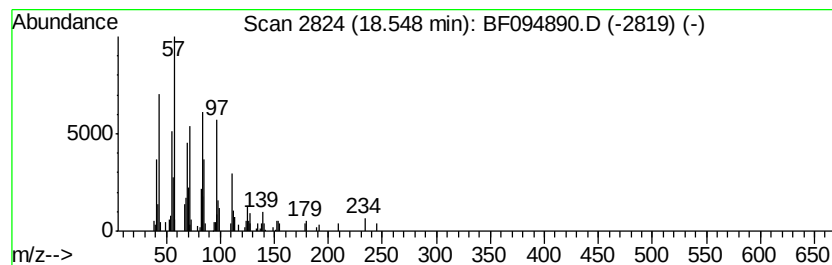
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Dotriacontyl heptafluorobut... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.55	4.21 ng	161068	Chrysene-d12	18.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	91
2		Octatriacontyl trifluoroacetate	647	C40H77F3O2	1000351-88-7	90
3		Triacontyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	87
4		Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	87
5		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	87



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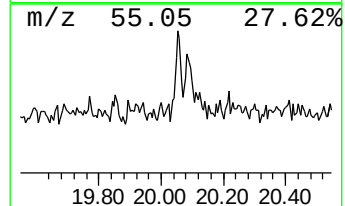
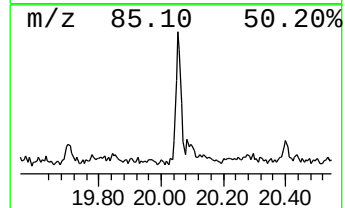
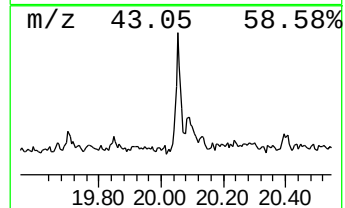
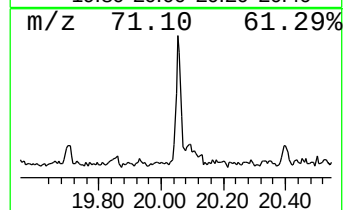
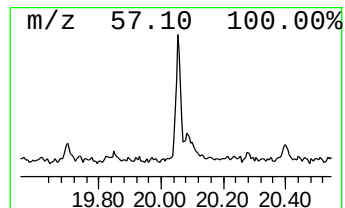
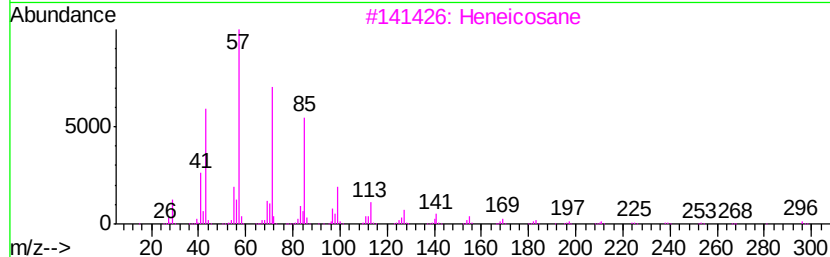
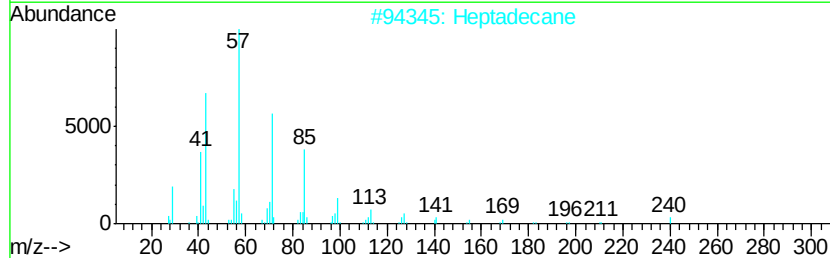
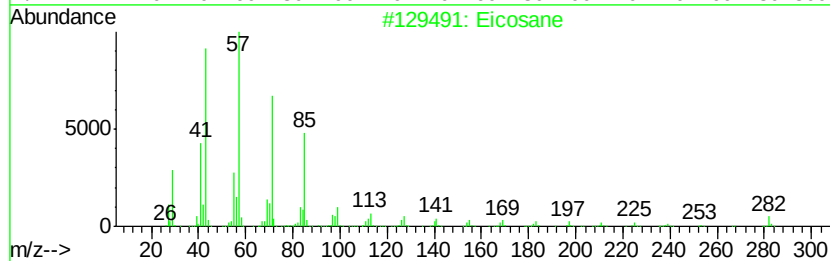
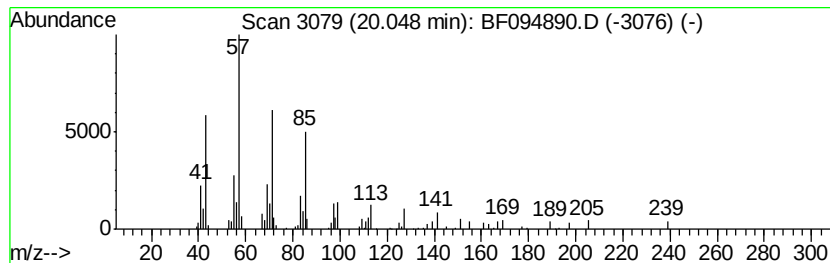
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.05	3.40 ng	101911	Perylene-d12	20.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	94
2		Heptadecane	240	C17H36	000629-78-7	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5		Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050417\
Data File : BF094890.D
Acq On : 4 May 2017 23:51
Operator : SJ/MA
Sample : I2930-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

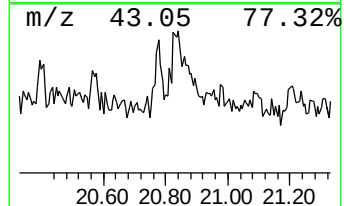
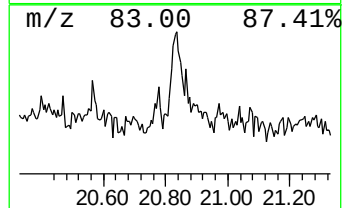
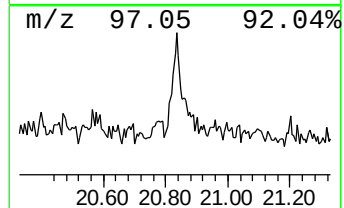
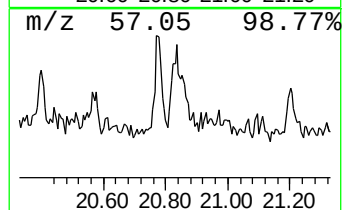
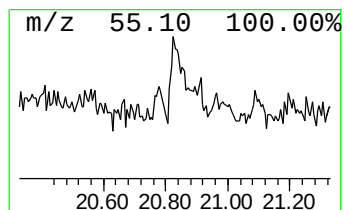
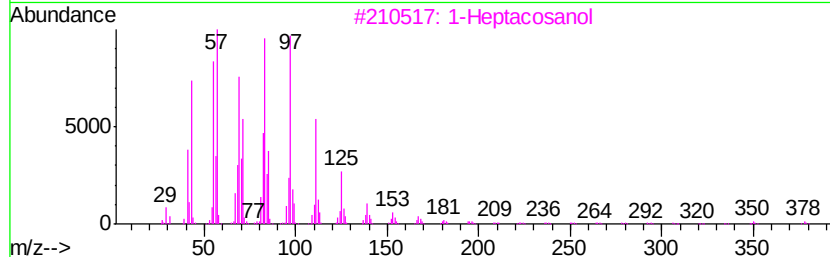
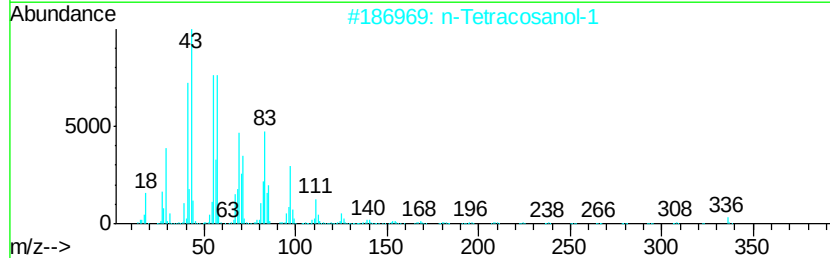
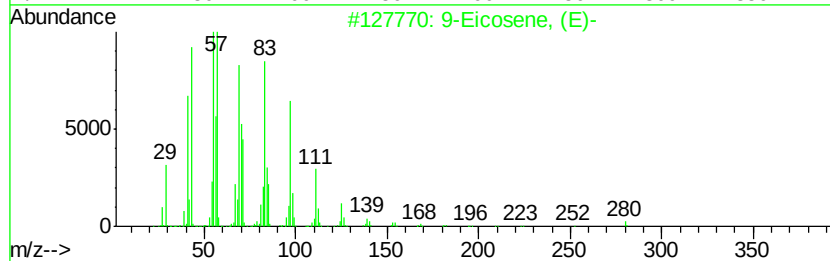
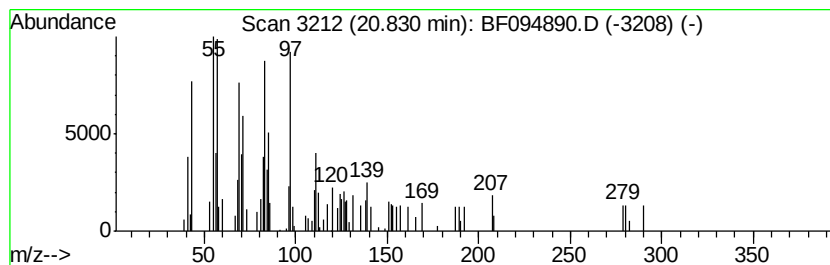
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BNA_F
ClientSampleId :
SP-1-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Eicosene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.83	2.60 ng	77896	Perylene-d12	20.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Eicosene, (E)-	280	C20H40	074685-29-3	90
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	83
3	1-Heptacosanol	396	C27H56O	002004-39-9	81
4	1-Eicosene	280	C20H40	003452-07-1	78
5	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	76



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050417\
Data File : BF094890.D
Acq On : 4 May 2017 23:51
Operator : SJ/MA
Sample : I2930-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1-COMP

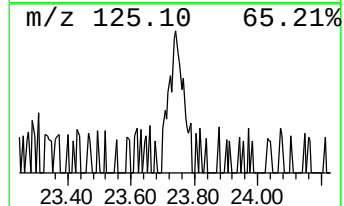
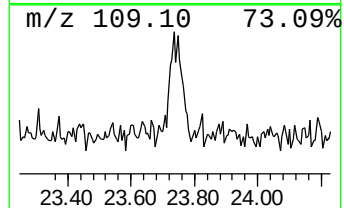
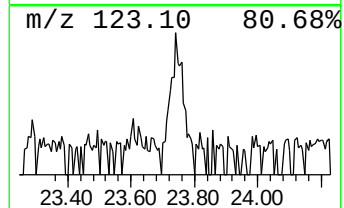
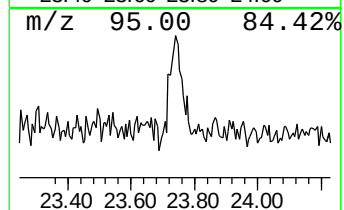
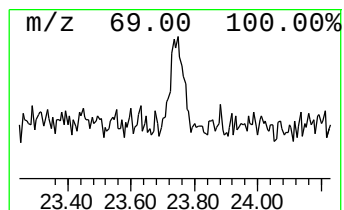
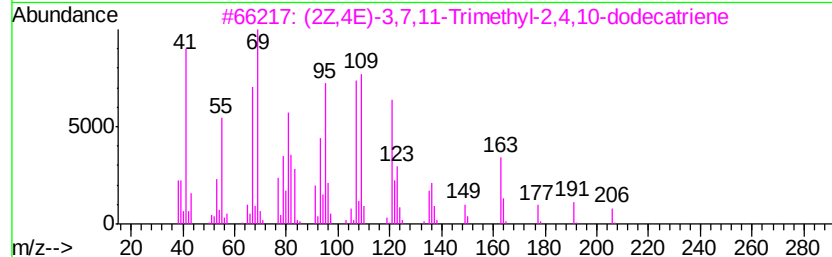
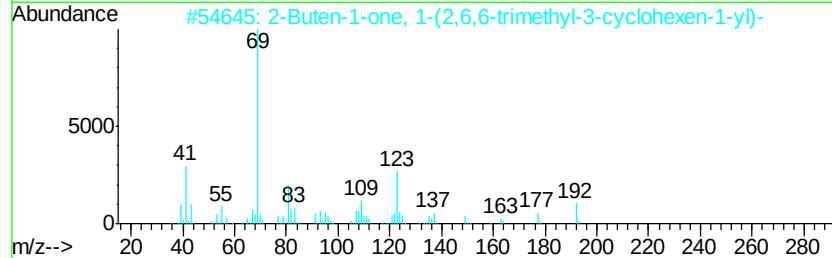
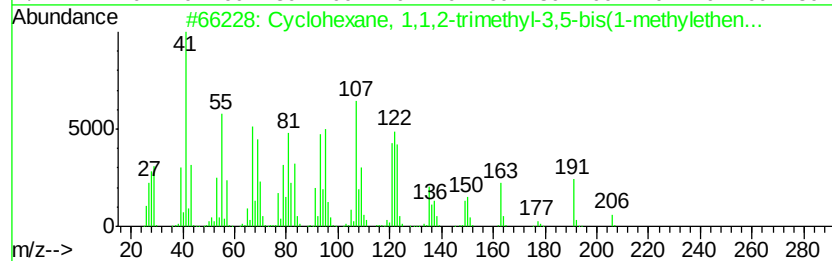
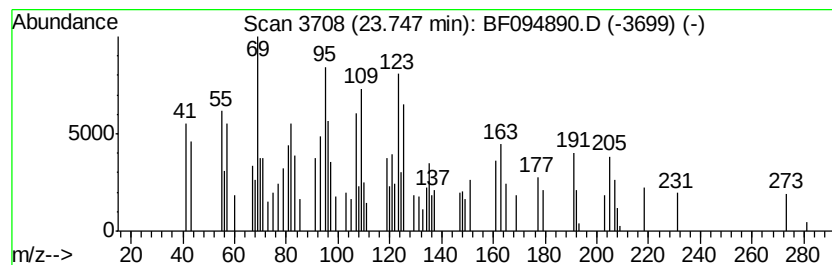
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cyclohexane, 1,1,2-trimethy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.75	3.66 ng	109521	Perylene-d12	20.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,1,2-trimethyl-3,5...	206	C15H26	062337-97-7	50
2			2-Buten-1-one, 1-(2,6,6-trimethy...	192	C13H20O	041436-42-4	35
3			(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	35
4			6-Isopropenyl-4,8a-dimethyl-4a,5...	218	C15H22O	086917-79-5	30
5			Alloaromadendrene oxide-(1)	220	C15H24O	1000156-12-8	27



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Sample : I2930-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.04	20.1	ng	530074	1	7.72	527438	20.0
unknown7.38	7.38	108.2	ng	2853990	1	7.72	527438	20.0
n-Hexadecanoic acid	15.94	6.5	ng	272296	4	14.97	834115	20.0
Dotriacontyl hept...	18.55	4.2	ng	161068	5	18.64	765191	20.0
Eicosane	20.05	3.4	ng	101911	6	20.29	599237	20.0
9-Eicosene, (E)-	20.83	2.6	ng	77896	6	20.29	599237	20.0
Cyclohexane, 1,1,...	23.75	3.7	ng	109521	6	20.29	599237	20.0