

Data Path : Z:\HPCHEM1\BNA G\DATA\BG102616\
 Data File : BG024517.D
 Acq On : 26 Oct 2016 18:13
 Operator : UM/SJ
 Sample : H5408-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-2

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_G\METHODS\8270-BG102516.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	5.337	418	425	432	rVB	84261	131370	4.58%	0.547%
2	5.795	498	503	515	rVB2	100461	190531	6.64%	0.794%
3	6.318	584	592	598	rBV6	15409	35867	1.25%	0.149%
4	7.405	770	777	778	rBV3	80435	125964	4.39%	0.525%
5	7.423	778	780	786	rVB2	81923	122201	4.26%	0.509%
6	7.793	836	843	852	rVB2	176552	306289	10.67%	1.276%
7	8.269	918	924	934	rBV	480846	853598	29.75%	3.556%
8	8.598	972	980	987	rBV2	426105	802924	27.98%	3.345%
9	9.444	1116	1124	1131	rBV2	445749	804881	28.05%	3.353%
10	9.791	1179	1183	1187	rBV3	42182	56821	1.98%	0.237%
11	11.101	1397	1406	1418	rBV	582321	1136418	39.60%	4.735%
12	13.510	1805	1816	1825	rVB	928653	1520297	52.98%	6.334%
13	14.321	1948	1954	1960	rBV	630595	959399	33.43%	3.997%
14	14.738	2019	2025	2031	rBV2	72336	103372	3.60%	0.431%
15	14.885	2042	2050	2058	rBV	927696	1523202	53.08%	6.346%
16	15.184	2096	2101	2106	rBV6	21970	38332	1.34%	0.160%
17	15.249	2106	2112	2114	rBV7	34067	56197	1.96%	0.234%
18	15.284	2116	2118	2124	rVV7	20387	33381	1.16%	0.139%
19	15.355	2125	2130	2136	rVV6	29403	49452	1.72%	0.206%
20	15.684	2180	2186	2192	rVB2	169814	244874	8.53%	1.020%
21	16.083	2248	2254	2259	rBV5	61366	137324	4.79%	0.572%
22	16.130	2259	2262	2266	rVV6	20813	31331	1.09%	0.131%
23	16.236	2274	2280	2284	rVB8	23919	39081	1.36%	0.163%
24	16.312	2289	2293	2296	rBV4	29848	40192	1.40%	0.167%
25	16.365	2296	2302	2309	rBV2	267145	443761	15.47%	1.849%
26	16.542	2328	2332	2343	rBV	214389	410354	14.30%	1.710%
27	16.712	2359	2361	2366	rVB5	23029	31710	1.11%	0.132%
28	16.894	2385	2392	2397	rBV8	35567	92182	3.21%	0.384%
29	17.123	2426	2431	2434	rBV5	20162	28721	1.00%	0.120%
30	17.335	2463	2467	2472	rBV2	125233	161391	5.62%	0.672%
31	17.388	2472	2476	2479	rBV6	27325	36307	1.27%	0.151%
32	17.629	2511	2517	2522	rBV	1245507	1971943	68.72%	8.216%
33	17.670	2522	2524	2531	rVB2	77483	95457	3.33%	0.398%
34	17.752	2536	2538	2544	rVB6	18942	34827	1.21%	0.145%

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35	18.075	2589	2593	2597	rBV6	36488	46522	1.62%	0.194%
36	18.475	2655	2661	2667	rBV	720605	1034671	36.06%	4.311%
37	18.551	2669	2674	2679	rVV9	35740	75366	2.63%	0.314%
38	18.698	2694	2699	2702	rBV7	17325	35109	1.22%	0.146%
39	18.892	2728	2732	2736	rBV6	55834	81898	2.85%	0.341%
40	19.074	2760	2763	2766	rVB5	35821	42109	1.47%	0.175%
41	19.221	2781	2788	2791	rVB9	25136	43848	1.53%	0.183%
42	19.338	2805	2808	2812	rVB5	37888	41862	1.46%	0.174%
43	19.485	2831	2833	2838	rVB6	21331	28887	1.01%	0.120%
44	19.591	2847	2851	2852	rBV4	59923	61651	2.15%	0.257%
45	19.656	2860	2862	2866	rVB2	49037	66430	2.32%	0.277%
46	19.697	2866	2869	2870	rBV3	43157	36634	1.28%	0.153%
47	19.732	2870	2875	2881	rVB	584636	758706	26.44%	3.161%
48	20.020	2922	2924	2928	rVB3	36876	47268	1.65%	0.197%
49	20.161	2943	2948	2951	rBV7	46987	82584	2.88%	0.344%
50	20.208	2951	2956	2962	rVB	1337394	1812996	63.18%	7.554%
51	20.343	2976	2979	2982	rBV5	25674	40236	1.40%	0.168%
52	20.413	2989	2991	2996	rVB3	73887	93400	3.25%	0.389%
53	20.795	3052	3056	3059	rBV5	32447	53411	1.86%	0.223%
54	20.848	3064	3065	3072	rVB7	42369	65066	2.27%	0.271%
55	20.978	3084	3087	3091	rVB6	40961	50213	1.75%	0.209%
56	21.518	3174	3179	3192	rBV2	391921	940352	32.77%	3.918%
57	21.765	3217	3221	3226	rVB2	96203	125251	4.36%	0.522%
58	21.924	3241	3248	3254	rVB	1477284	2662464	92.79%	11.093%
59	23.116	3449	3451	3454	rVB4	40203	40957	1.43%	0.171%
60	25.355	3821	3832	3844	rVB2	958318	2869448	100.00%	11.955%
61	26.524	4026	4031	4041	rBV2	29111	82040	2.86%	0.342%
62	26.671	4053	4056	4057	rBV3	26644	31909	1.11%	0.133%

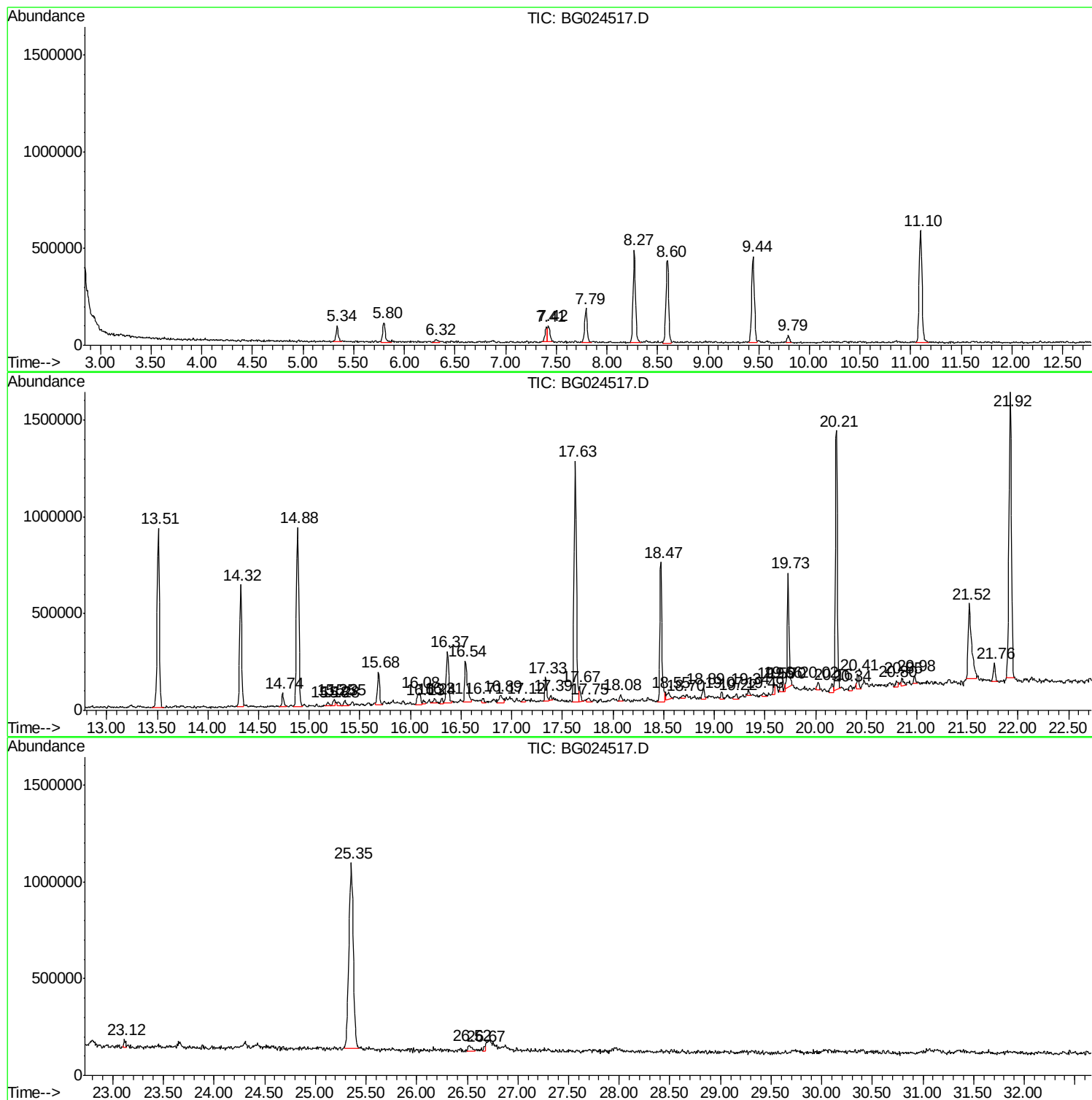
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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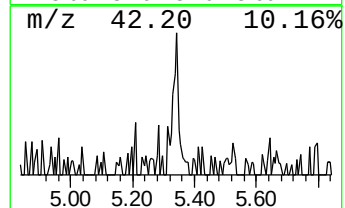
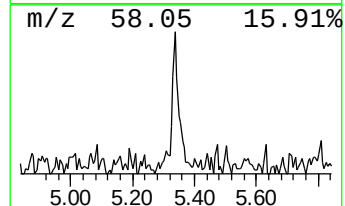
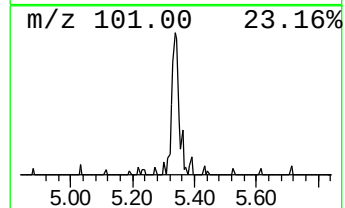
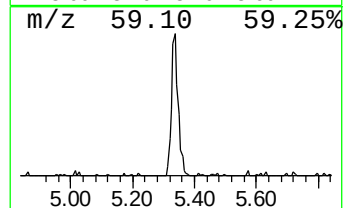
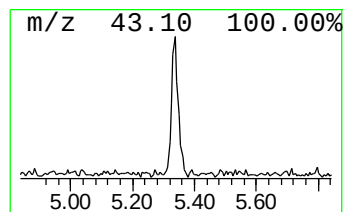
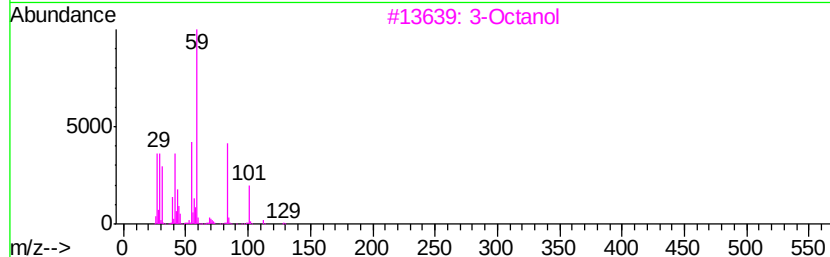
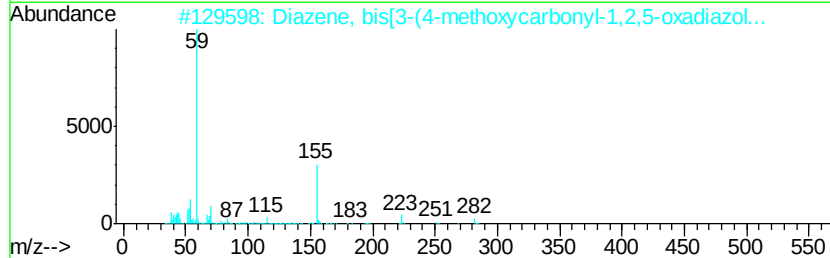
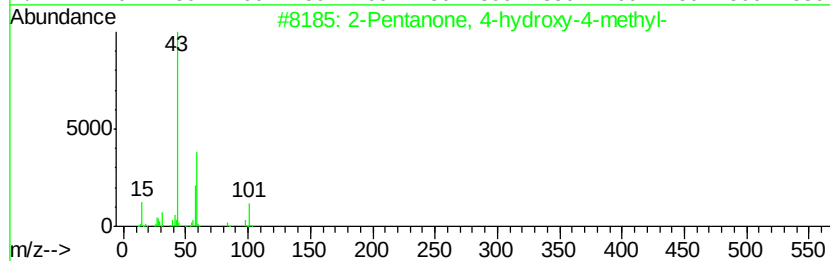
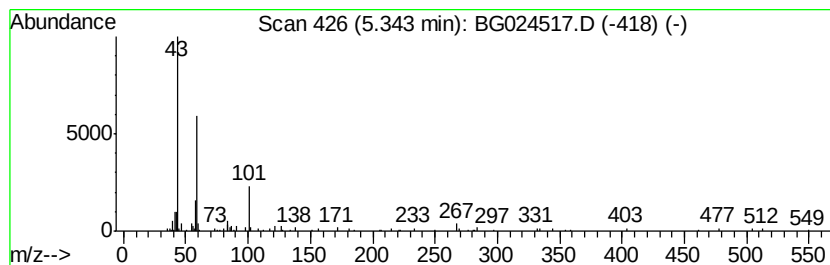
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.34	3.08 ng	131370	1,4-Dichlorobenzene-d4	8.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Diazene, bis[3-(4-methoxycarbonyl-1,2,5-oxadiazol-5-yl)-	282	C8H6N6O6	339246-68-3	43
3		3-Octanol	130	C8H18O	000589-98-0	36
4		3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	36
5		Cycloserine	102	C3H6N2O2	000068-41-7	25



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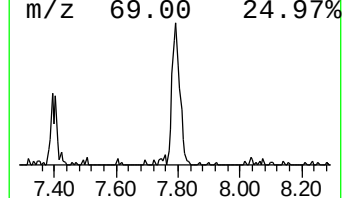
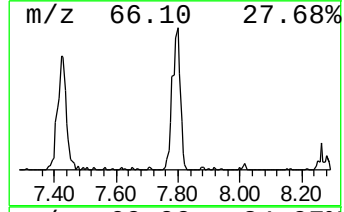
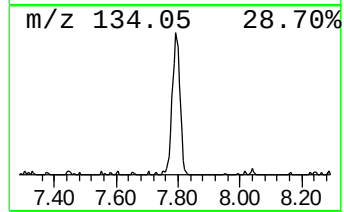
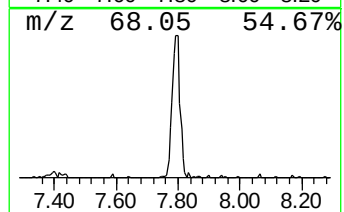
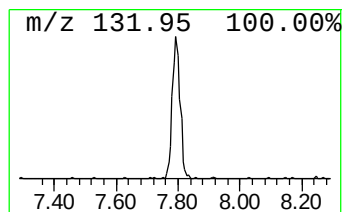
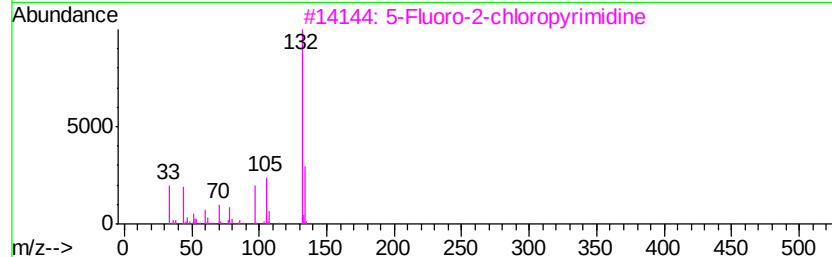
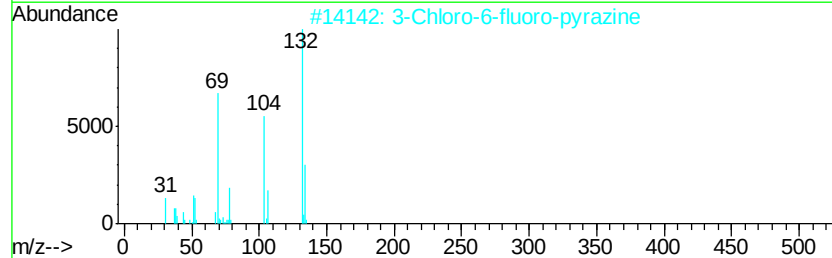
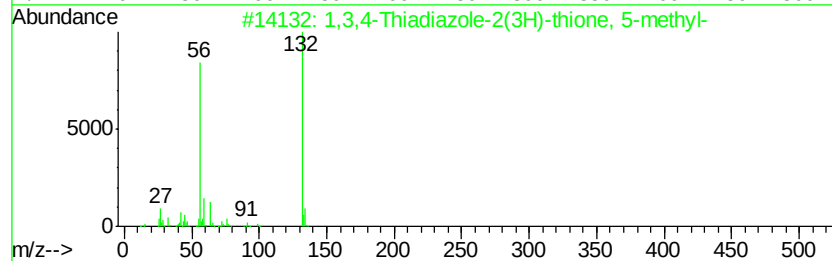
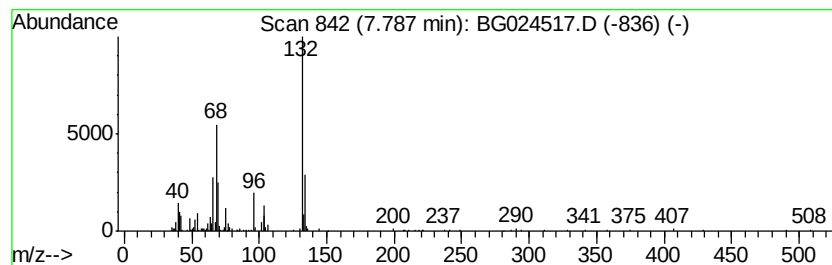
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.79 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	7.18 ng	306289	1,4-Dichlorobenzene-d4	8.27

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	22
2			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	22
3			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	22
4			5-Aminoindole	132	C8H8N2	005192-03-0	12
5			1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12



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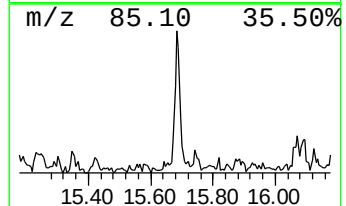
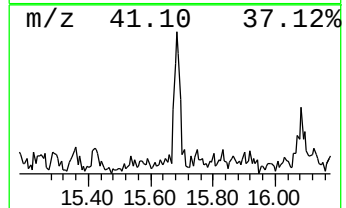
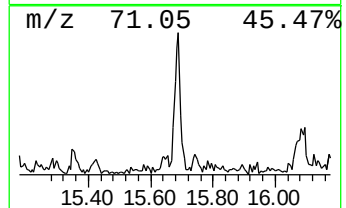
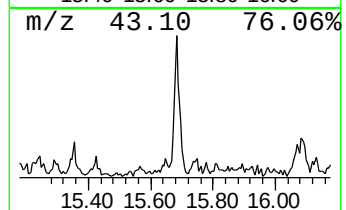
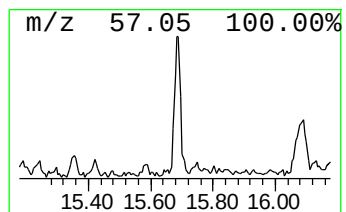
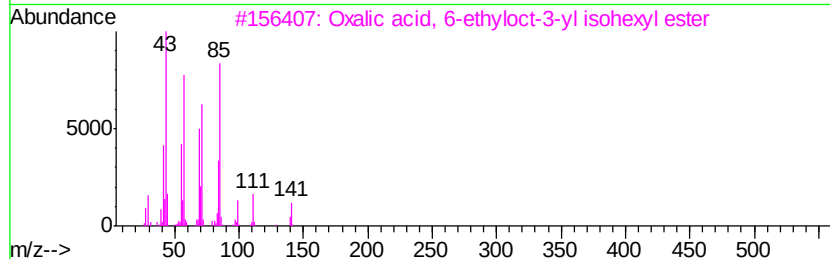
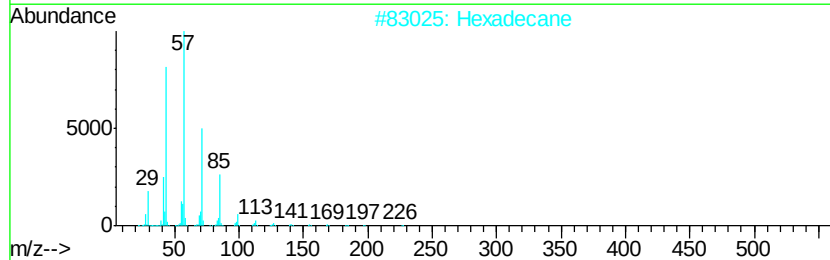
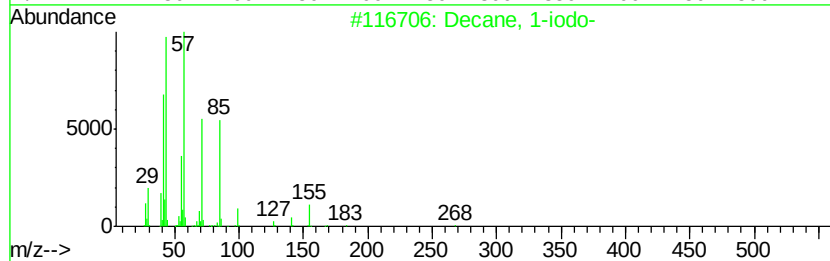
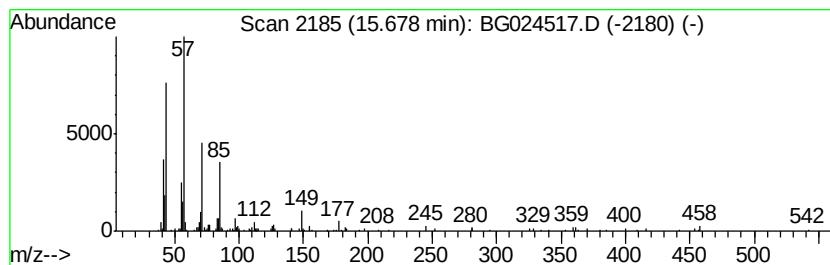
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Decane, 1-iodo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.68	3.22 ng	244874	Acenaphthene-d10	14.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decane, 1-iodo-	268	C10H21I	002050-77-3	83
2		Hexadecane	226	C16H34	000544-76-3	64
3		Oxalic acid, 6-ethvloct-3-vl iso...	314	C18H34O4	1000309-34-3	59
4		Tridecane	184	C13H28	000629-50-5	58
5		Octadecane, 5-methyl-	268	C19H40	025117-35-5	53



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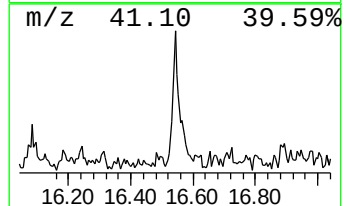
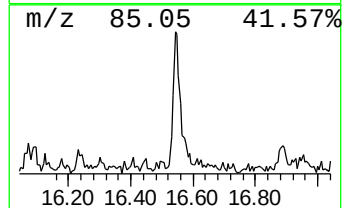
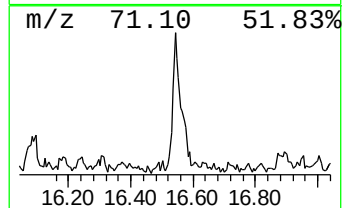
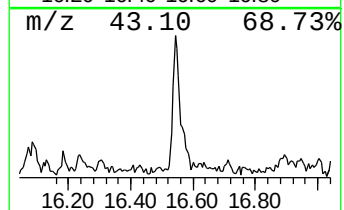
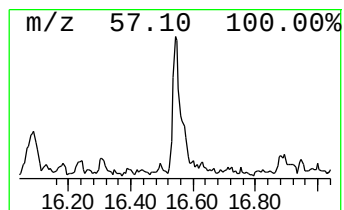
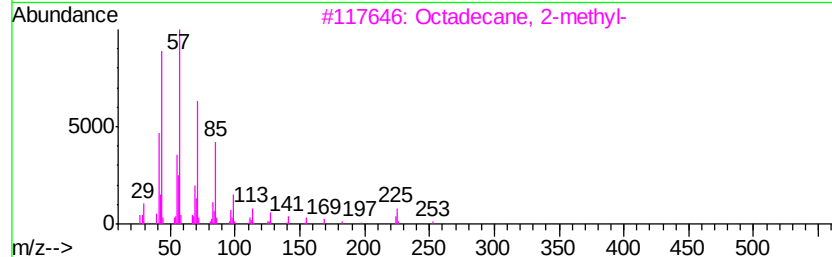
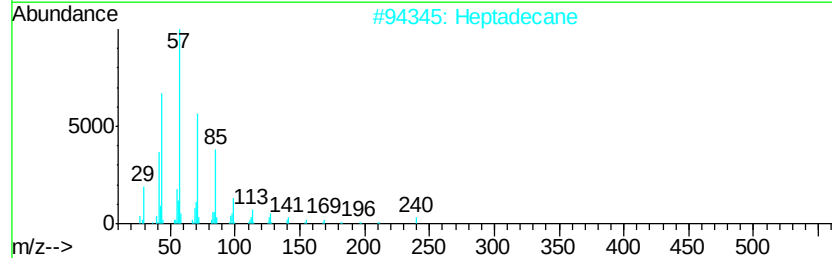
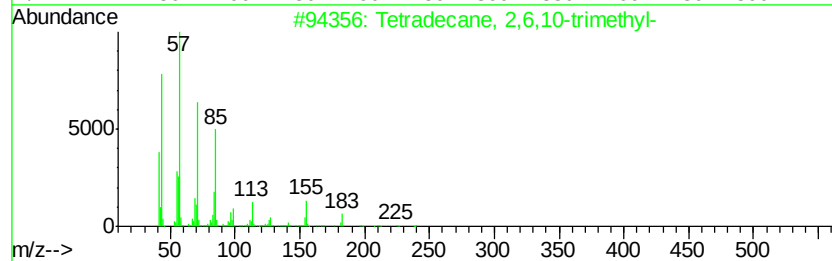
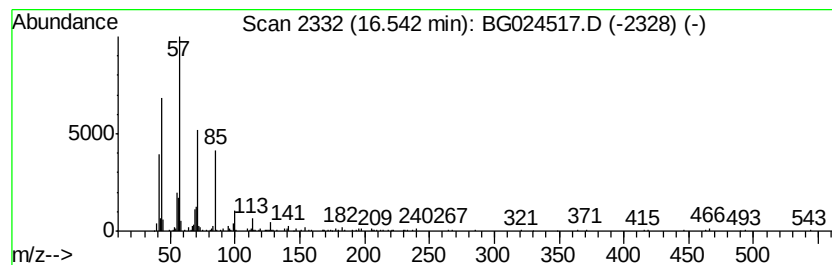
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tetradecane, 2,6,10-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.54	4.16 ng	410354	Phenanthrene-d10	17.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	87
2		Heptadecane	240	C17H36	000629-78-7	83
3		Octadecane, 2-methyl-	268	C19H40	001560-88-9	80
4		Hexadecane	226	C16H34	000544-76-3	80
5		Tetracosane	338	C24H50	000646-31-1	80



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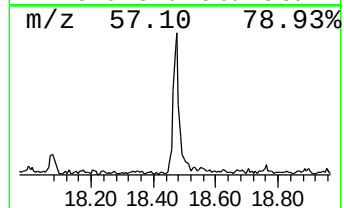
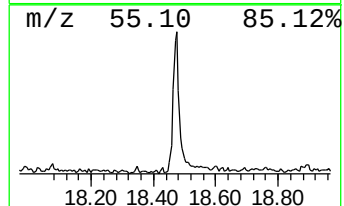
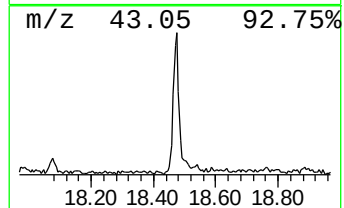
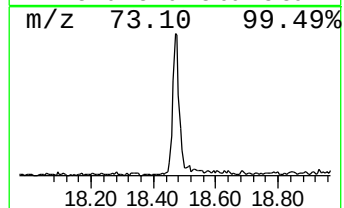
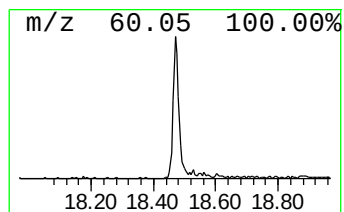
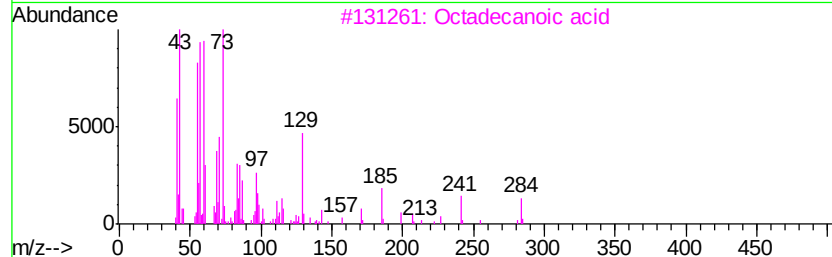
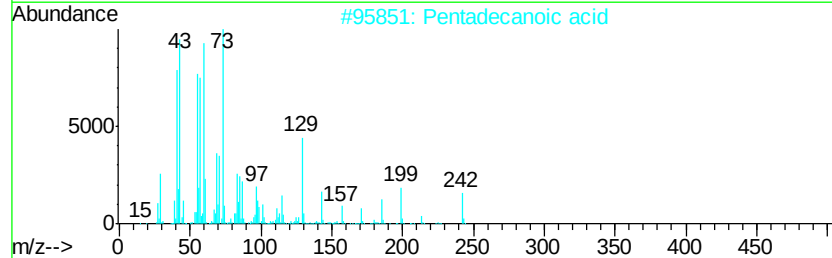
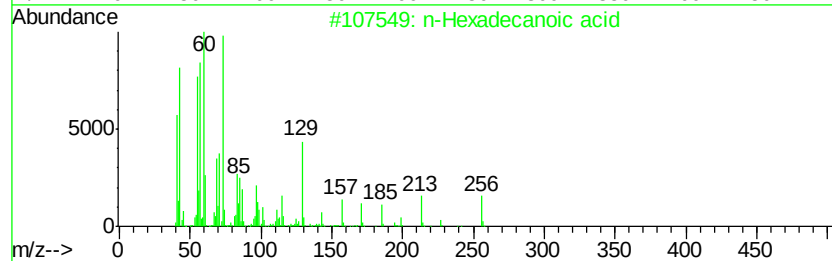
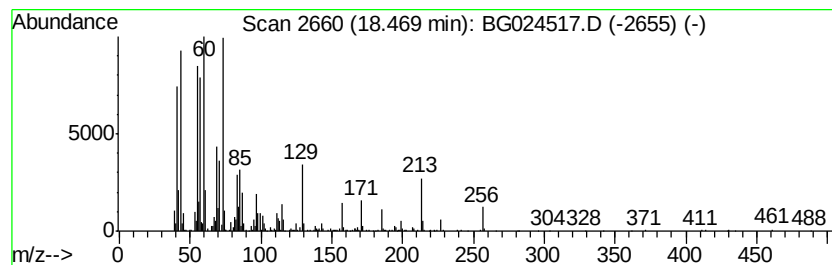
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.47	10.49 ng	1034670	Phenanthrene-d10	17.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3		Octadecanoic acid	284	C18H36O2	000057-11-4	64
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5		Tridecanoic acid	214	C13H26O2	000638-53-9	58



Data Path : Z:\HPCHEM1\BNA G\DATA\BG102616\
Data File : BG024517.D
Acq On : 26 Oct 2016 18:13
Operator : UM/SJ
Sample : H5408-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-2

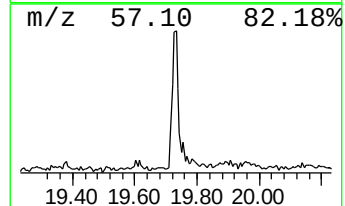
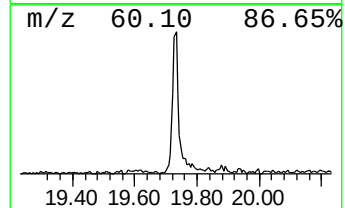
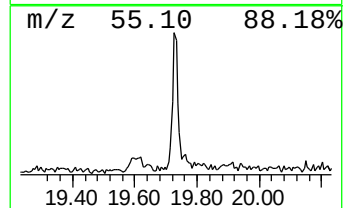
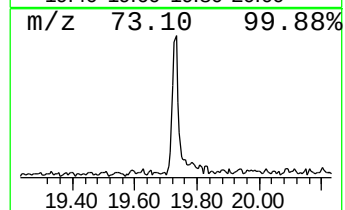
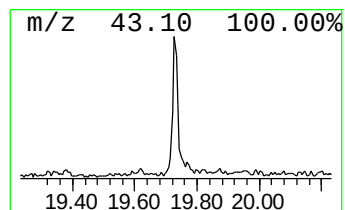
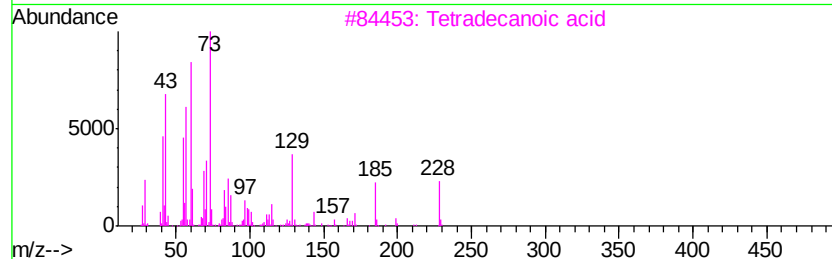
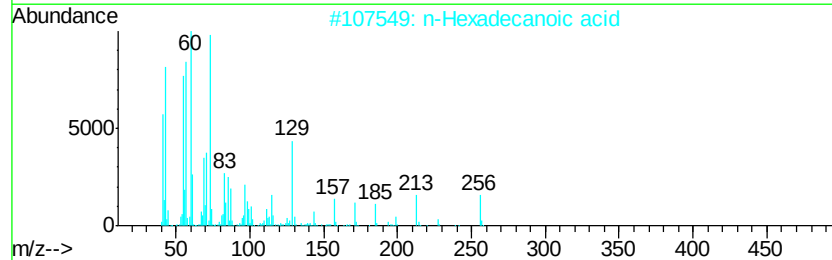
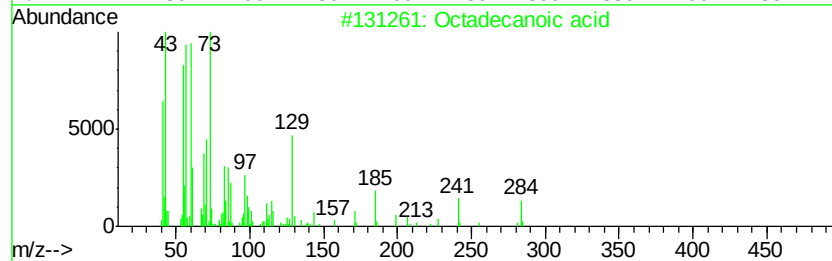
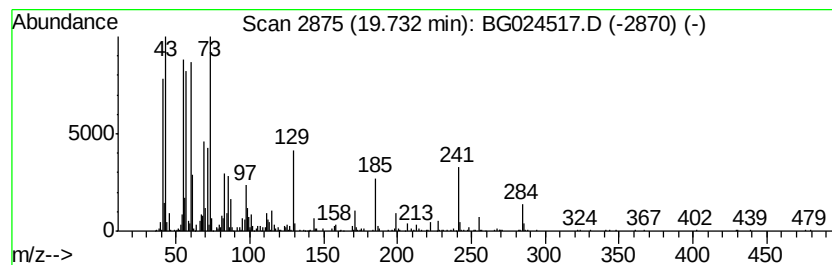
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.73	7.70 ng	758706	Phenanthrene-d10	17.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4		n-Decanoic acid	172	C10H20O2	000334-48-5	64
5		Tridecanoic acid	214	C13H26O2	000638-53-9	53



Data Path : Z:\HPCHEM1\BNA G\DATA\BG102616\
Data File : BG024517.D
Acq On : 26 Oct 2016 18:13
Operator : UM/SJ
Sample : H5408-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-2

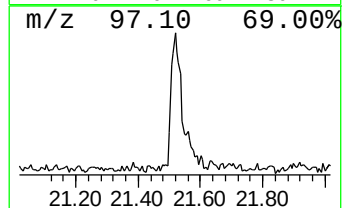
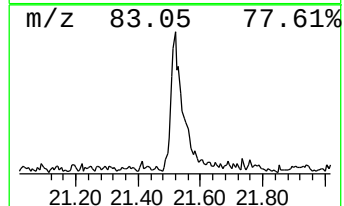
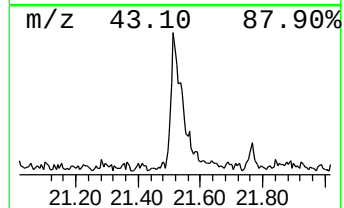
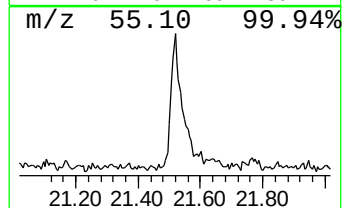
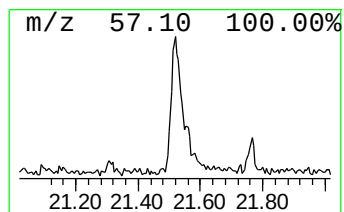
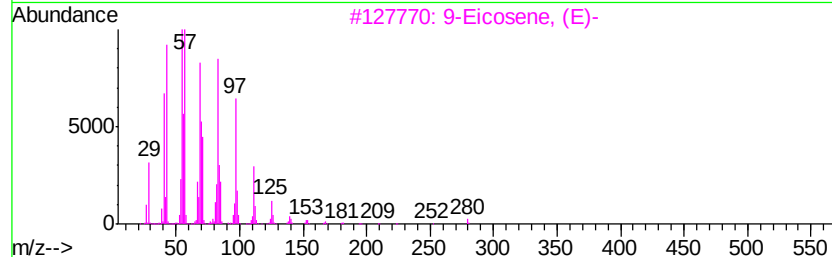
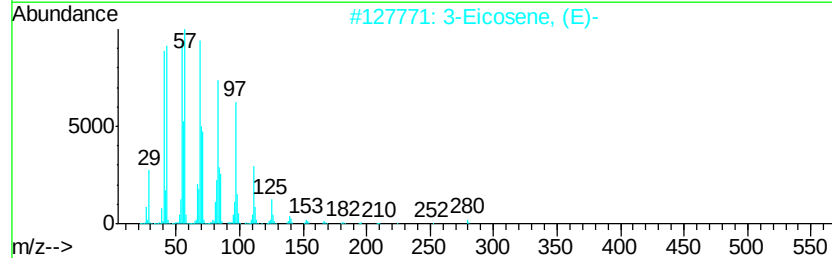
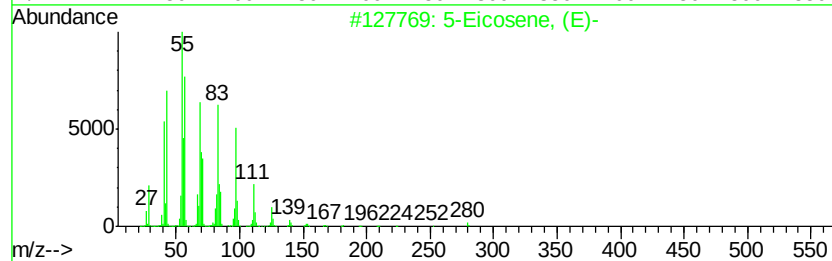
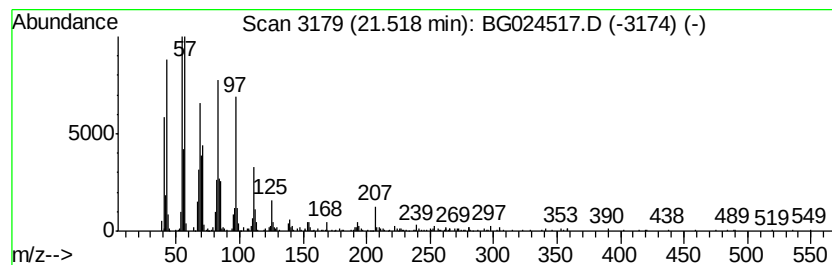
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 5-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.52	7.06 ng	940352	Chrysene-d12	21.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	98
3		9-Eicosene, (E)-	280	C20H40	074685-29-3	95
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
5		1-Eicosene	280	C20H40	003452-07-1	94



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG102616\
Data File : BG024517.D
Acq On : 26 Oct 2016 18:13
Operator : UM/SJ
Sample : H5408-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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...	5.34	3.1 ng		131370	1	8.27	853598	20.0
unknown7.79	7.79	7.2 ng		306289	1	8.27	853598	20.0
Decane, 1-iodo-	15.68	3.2 ng		244874	3	14.88	1523200	20.0
Tetradecane, 2,6,...	16.54	4.2 ng		410354	4	17.63	1971940	20.0
n-Hexadecanoic acid	18.47	10.5 ng		1034670	4	17.63	1971940	20.0
Octadecanoic acid	19.73	7.7 ng		758706	4	17.63	1971940	20.0
5-Eicosene, (E)-	21.52	7.1 ng		940352	5	21.92	2662460	20.0