

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051517\
 Data File : BM010041.D
 Acq On : 15 May 2017 15:54
 Operator : SJ/MA
 Sample : I3100-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PMW-2-051017

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_M\METHODS\8270-BM051117.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	4.899	303	308	316	rVB2	36425	59261	3.34%	0.412%
2	5.352	379	385	397	rBV	278234	452534	25.51%	3.145%
3	6.940	647	655	667	rBV2	195236	427390	24.09%	2.970%
4	7.293	709	715	728	rBV2	448173	729937	41.14%	5.072%
5	7.628	767	772	781	rVB4	24656	47812	2.70%	0.332%
6	7.757	788	794	801	rBV	299723	469554	26.47%	3.263%
7	7.893	811	817	822	rBV4	14830	25564	1.44%	0.178%
8	8.075	842	848	858	rVB2	558557	898489	50.65%	6.244%
9	8.510	917	922	929	rBV5	17455	35783	2.02%	0.249%
10	8.681	947	951	956	rBV3	12103	21394	1.21%	0.149%
11	8.793	965	970	973	rBV3	21469	36939	2.08%	0.257%
12	8.934	985	994	1008	rBV	438413	825613	46.54%	5.737%
13	9.063	1011	1016	1022	rVV6	11829	24433	1.38%	0.170%
14	9.175	1029	1035	1038	rBV5	13689	21258	1.20%	0.148%
15	9.304	1053	1057	1063	rVB4	8721	17819	1.00%	0.124%
16	10.551	1262	1269	1279	rBV	331486	565148	31.86%	3.927%
17	11.210	1376	1381	1384	rBV4	16072	26453	1.49%	0.184%
18	11.851	1484	1490	1499	rBV3	22534	43999	2.48%	0.306%
19	12.239	1546	1556	1565	rBV	444779	854542	48.17%	5.938%
20	13.022	1683	1689	1695	rBV	957130	1367650	77.09%	9.504%
21	13.869	1827	1833	1843	rBV	281620	403031	22.72%	2.801%
22	14.280	1897	1903	1909	rBV2	30357	40585	2.29%	0.282%
23	14.410	1918	1925	1934	rVB2	404958	630453	35.54%	4.381%
24	14.898	2004	2008	2015	rVB2	12338	18368	1.04%	0.128%
25	15.233	2061	2065	2070	rBV3	81310	102074	5.75%	0.709%
26	15.633	2124	2133	2138	rBV4	26234	63430	3.58%	0.441%
27	15.786	2155	2159	2163	rBV3	11497	18631	1.05%	0.129%
28	15.916	2175	2181	2188	rBV	473169	720872	40.63%	5.009%
29	16.098	2206	2212	2224	rBV2	109507	212344	11.97%	1.476%
30	16.439	2267	2270	2273	rBV5	13463	18000	1.01%	0.125%
31	16.563	2286	2291	2294	rBV3	13688	20159	1.14%	0.140%
32	16.668	2304	2309	2313	rBV	94785	123011	6.93%	0.855%
33	16.892	2343	2347	2351	rBV	60730	76256	4.30%	0.530%
34	16.933	2351	2354	2358	rVB4	14319	22957	1.29%	0.160%

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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

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35	17.168	2387	2394	2403	rBV	471637	717722	40.46%	4.988%
36	17.627	2469	2472	2477	rBV3	19940	21818	1.23%	0.152%
37	17.927	2517	2523	2528	rBV7	15146	33041	1.86%	0.230%
38	18.045	2538	2543	2555	rBV	167004	254341	14.34%	1.767%
39	19.321	2757	2760	2766	rBV3	82025	118343	6.67%	0.822%
40	19.492	2786	2789	2794	rVB6	15730	21388	1.21%	0.149%
41	19.792	2834	2840	2845	rBV	1464078	1774082	100.00%	12.328%
42	20.580	2972	2974	2977	rVB4	23841	22975	1.30%	0.160%
43	21.045	3050	3053	3060	rVB2	132939	190942	10.76%	1.327%
44	21.356	3101	3106	3114	rBV	663126	939301	52.95%	6.527%
45	21.939	3203	3205	3206	rBV	30880	24373	1.37%	0.169%
46	23.650	3490	3496	3506	rVB	425586	850169	47.92%	5.908%

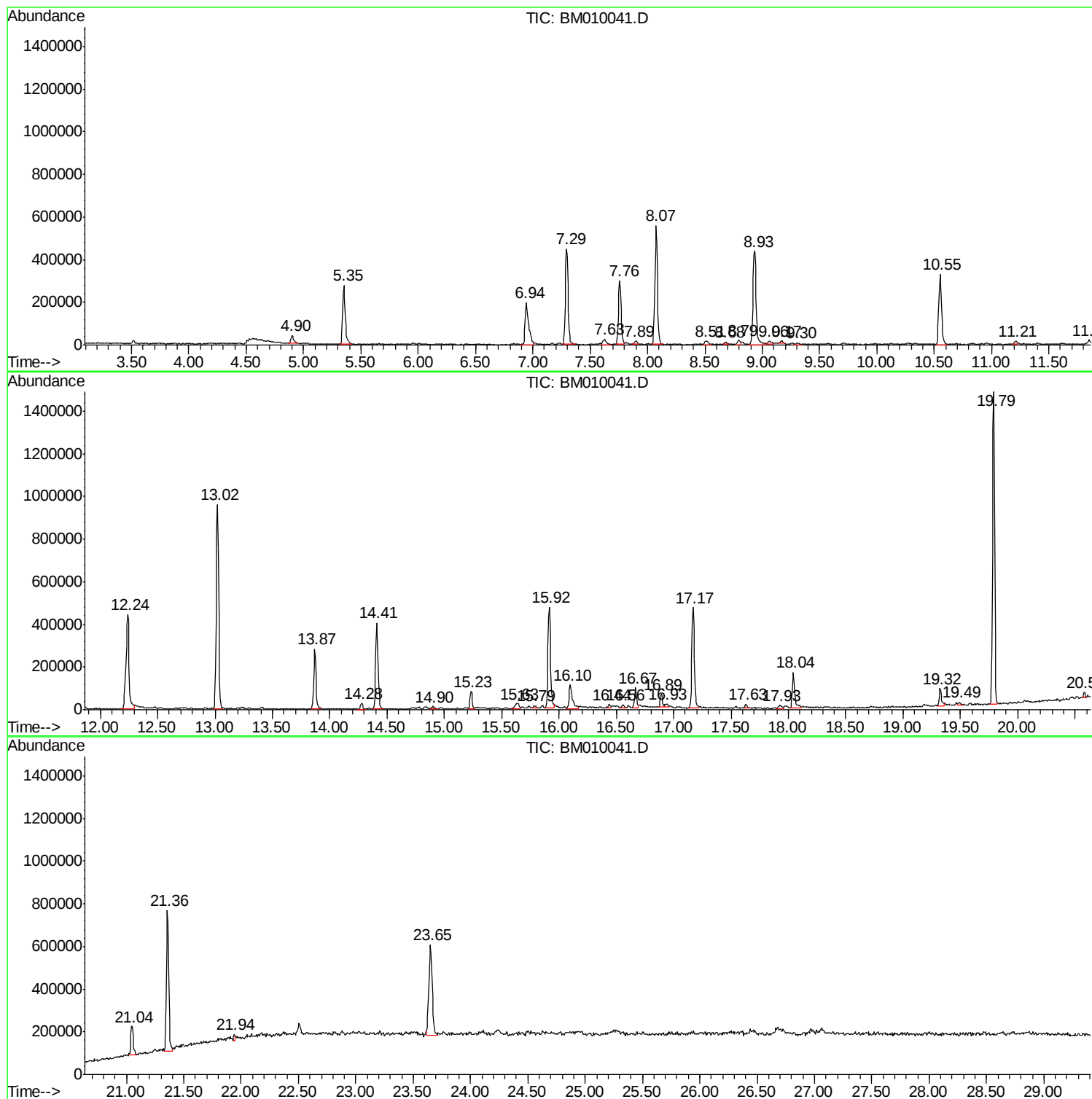
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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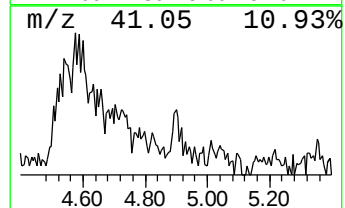
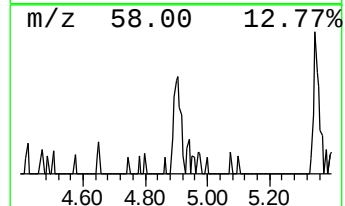
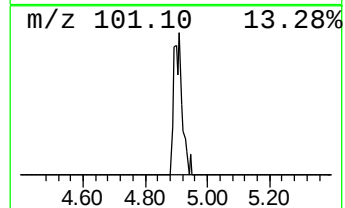
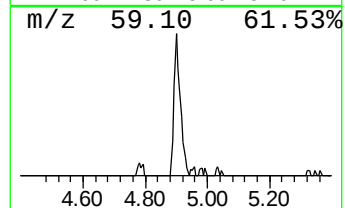
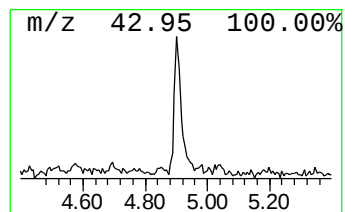
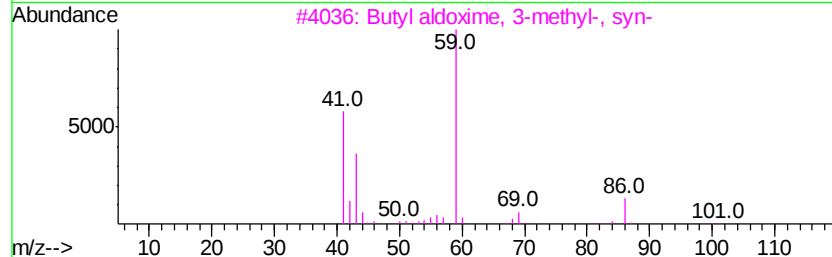
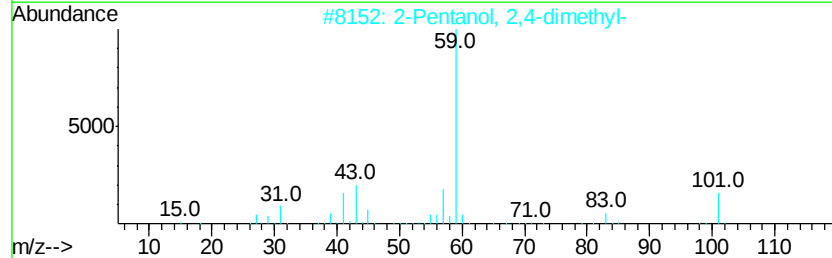
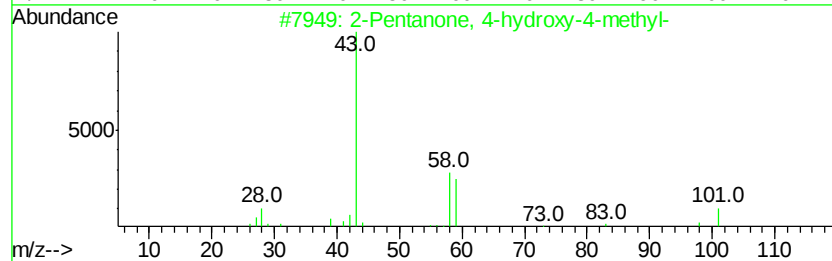
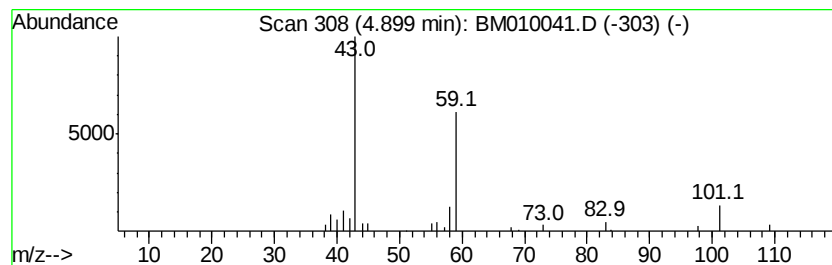
Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	2.52 ng	59261	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	33
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9



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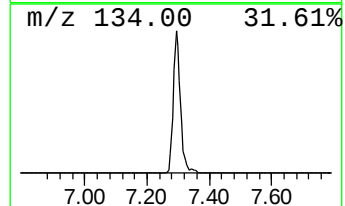
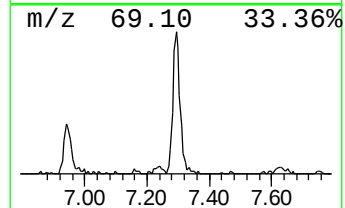
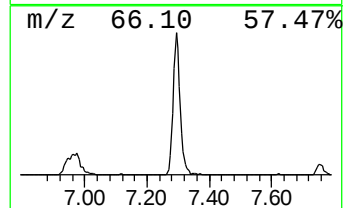
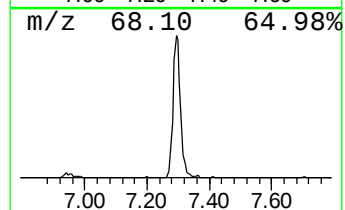
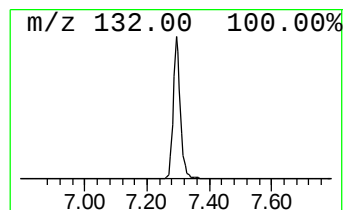
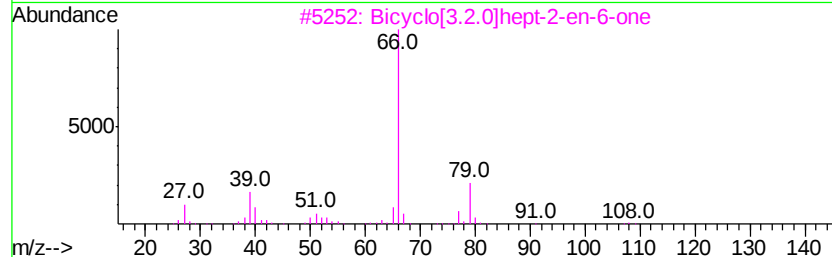
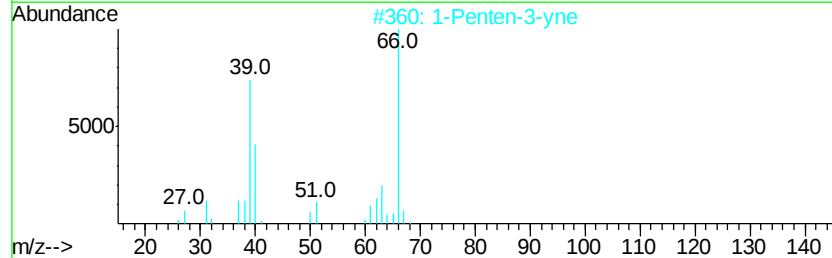
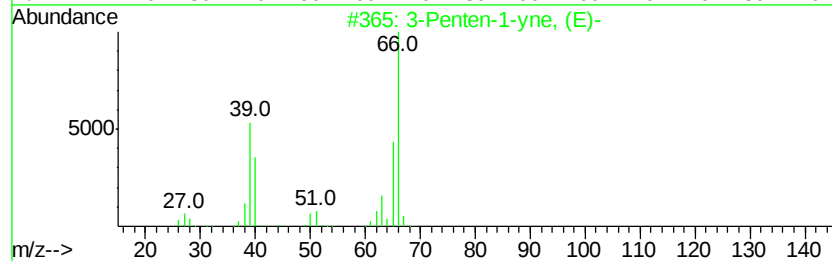
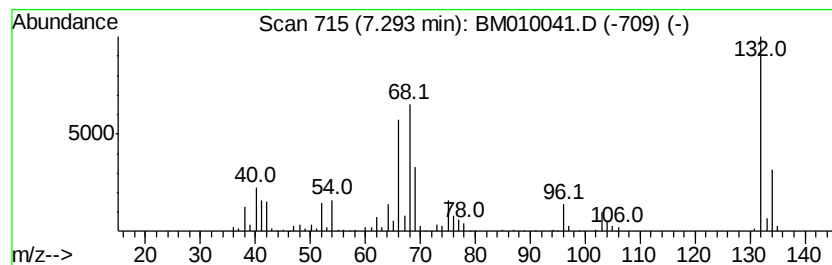
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.29 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.29	31.09 ng	729937	1,4-Dichlorobenzene-d4	7.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-1-yne, (E)-	66	C5H6	002004-69-5	35
2		1-Penten-3-yne	66	C5H6	000646-05-9	35
3		Bicyclo[3.2.0]hept-2-en-6-one	108	C7H8O	013173-09-6	25
4		Silane, bicyclo[2.2.1]hept-5-en-...	226	C7H9Cl3Si	014319-64-3	25
5		Bicyclo[2.2.1]hept-5-ene-2-aceti...	180	C11H16O2	074876-17-8	25



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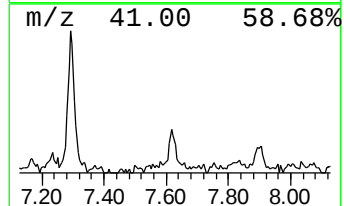
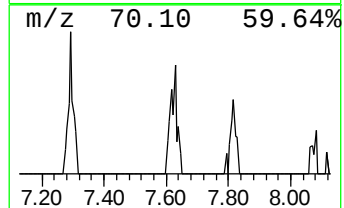
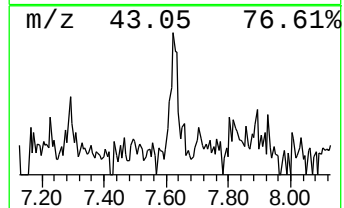
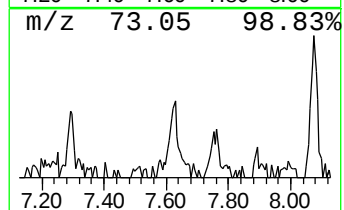
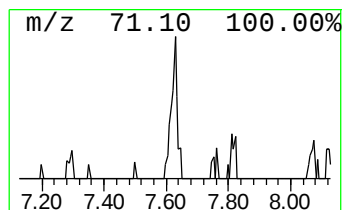
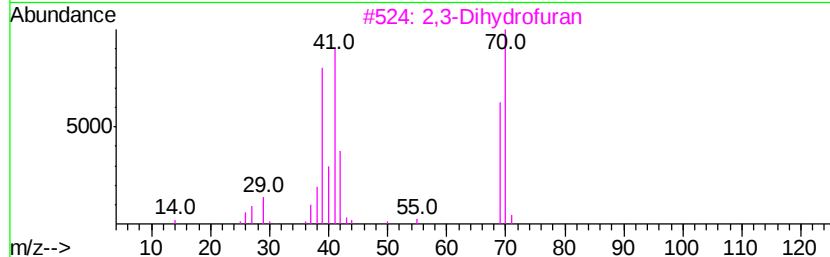
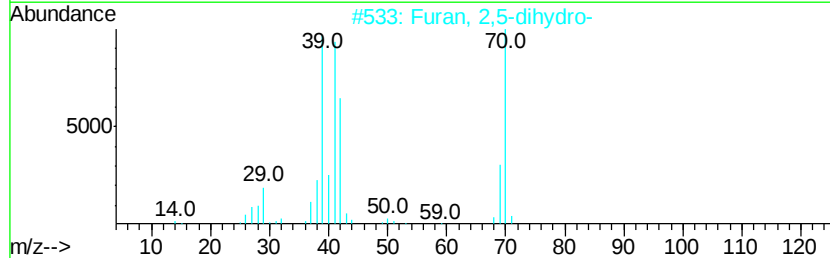
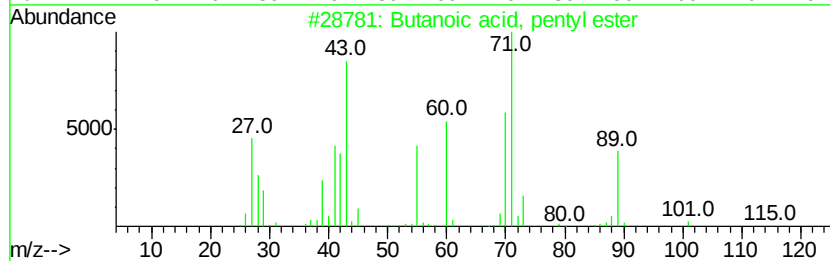
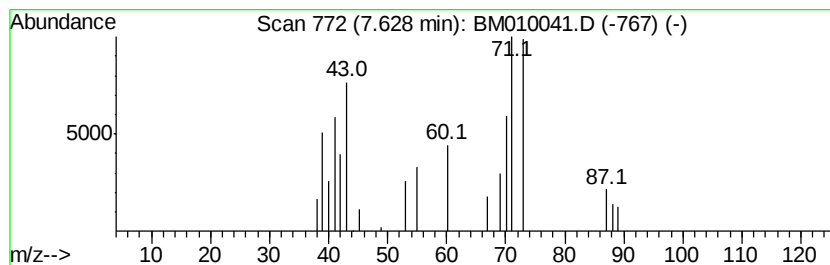
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown7.63 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.63	2.04 ng	47812	1,4-Dichlorobenzene-d4	7.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	47
2		Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	25
3		2,3-Dihydrofuran	70	C4H6O	001191-99-7	14
4		Pentane, 2-chloro-	106	C5H11Cl	000625-29-6	14
5		2-Butenal	70	C4H6O	004170-30-3	14



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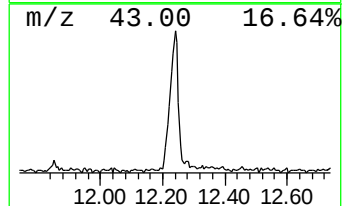
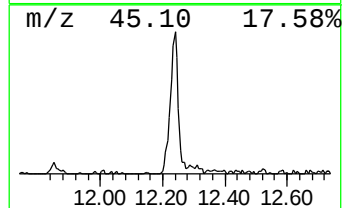
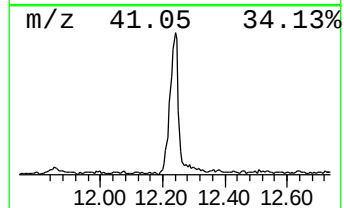
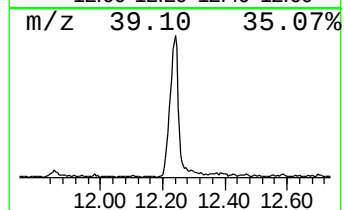
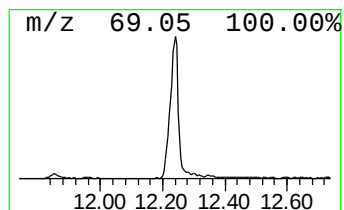
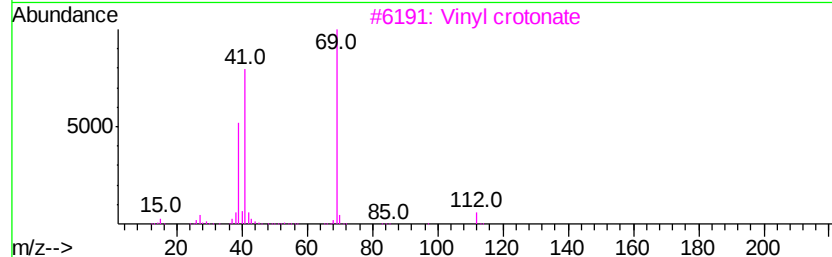
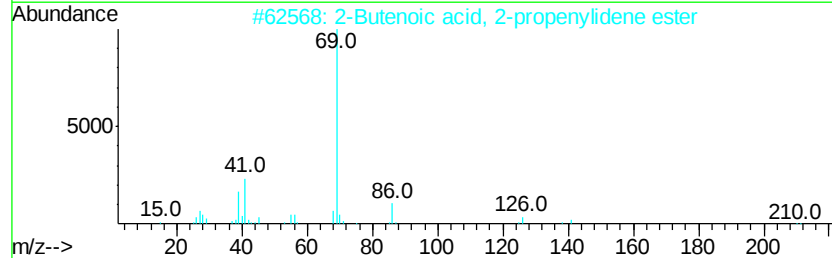
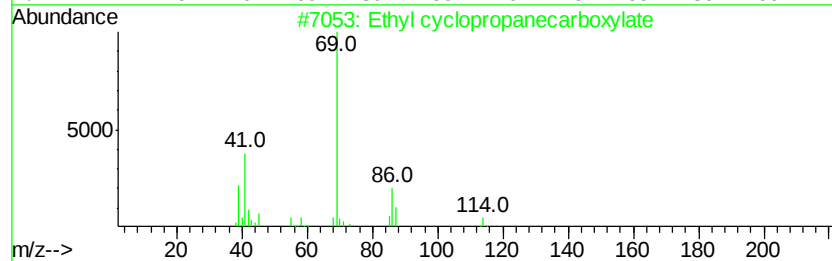
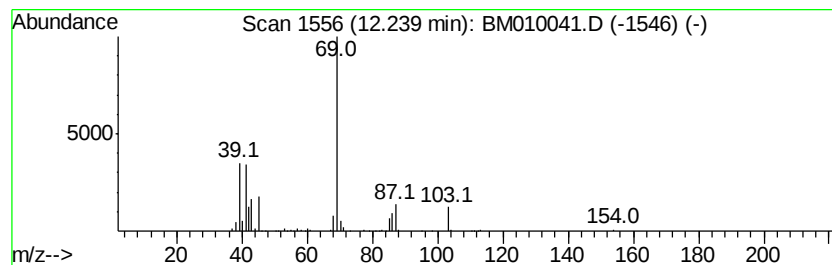
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Ethyl cyclopropanecarboxylate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.24	30.24 ng	854542	Naphthalene-d8	10.55

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	50
2		2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	42
3		Vinyl crotonate	112	C6H8O2	014861-06-4	28
4		Oxazole	69	C3H3NO	000288-42-6	9
5		Isoxazole	69	C3H3NO	000288-14-2	9



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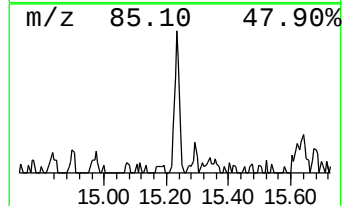
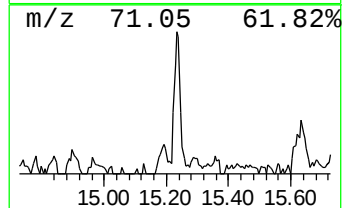
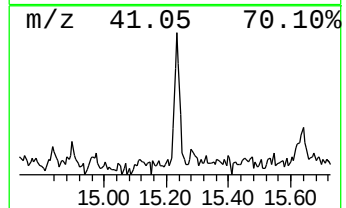
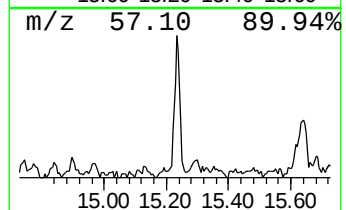
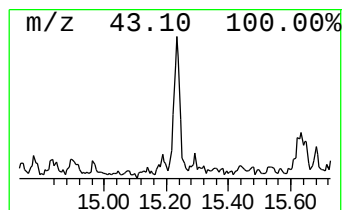
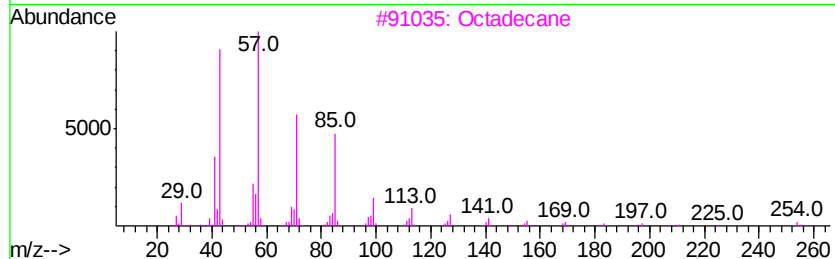
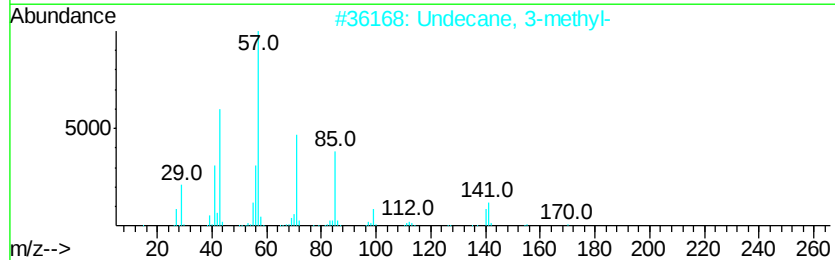
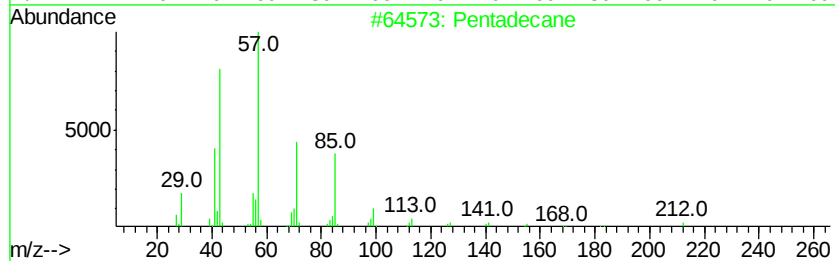
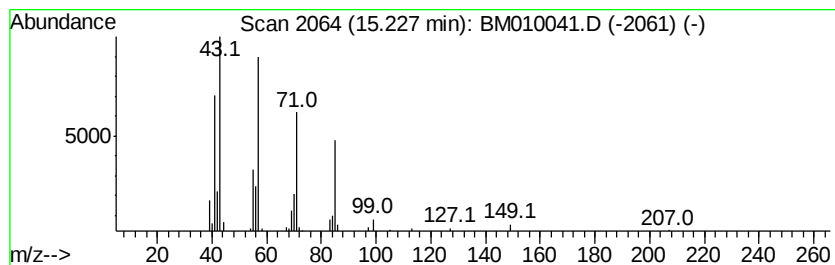
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Pentadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.23	3.24 ng	102074	Acenaphthene-d10	14.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane		212	C15H32	000629-62-9	72
2	Undecane, 3-methyl-		170	C12H26	001002-43-3	72
3	Octadecane		254	C18H38	000593-45-3	64
4	Silane, trichlorooctadecyl-		386	C18H37Cl3Si	000112-04-9	64
5	Decane, 1-iodo-		268	C10H21I	002050-77-3	64



Data Path : Z:\HPCHEM1\BNA M\DATA\BM051517\
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Acq On : 15 May 2017 15:54
Operator : SJ/MA
Sample : I3100-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

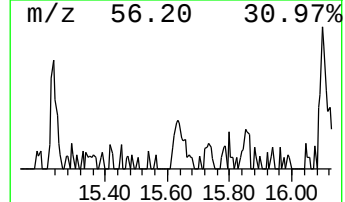
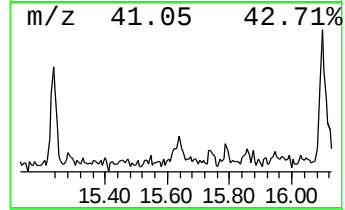
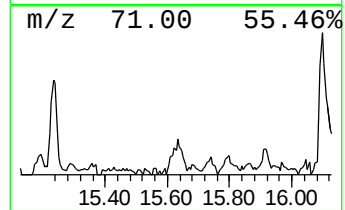
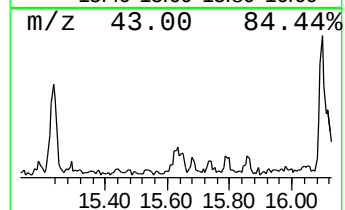
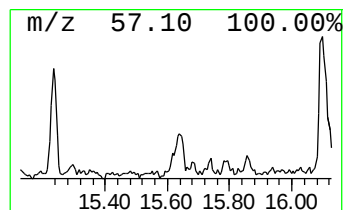
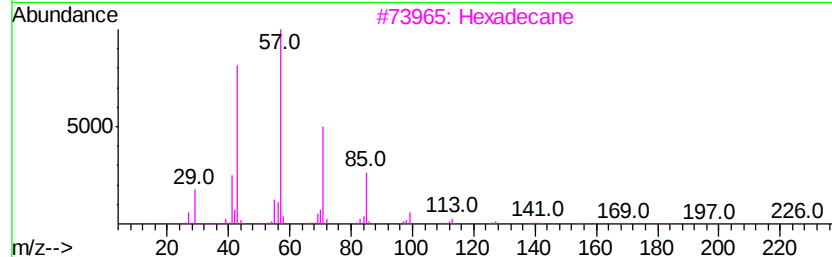
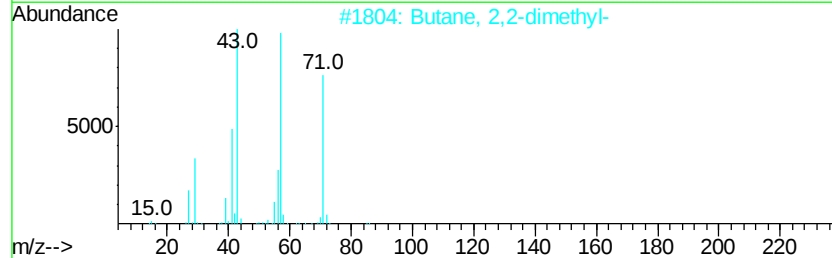
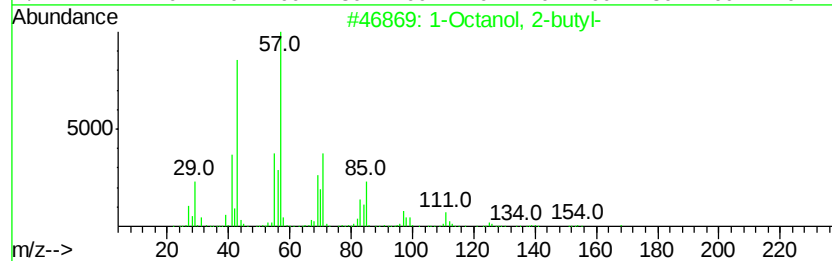
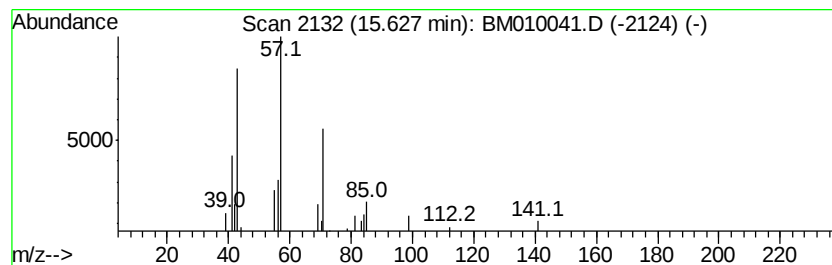
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Octanol, 2-butyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.63	2.01 ng	63430	Acenaphthene-d10	14.41
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Octanol, 2-butyl-	186 C12H26O	003913-02-8	53
2	Butane, 2,2-dimethyl-	86 C6H14	000075-83-2	43
3	Hexadecane	226 C16H34	000544-76-3	42
4	Decane, 2,5,6-trimethyl-	184 C13H28	062108-23-0	40
5	Decane, 2,5,9-trimethyl-	184 C13H28	062108-22-9	37



Data Path : Z:\HPCHEM1\BNA M\DATA\BM051517\
Data File : BM010041.D
Acq On : 15 May 2017 15:54
Operator : SJ/MA
Sample : I3100-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

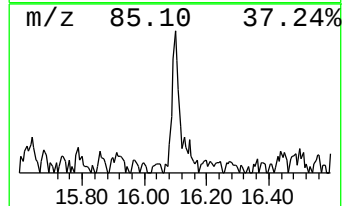
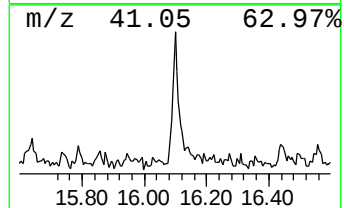
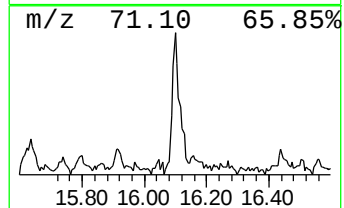
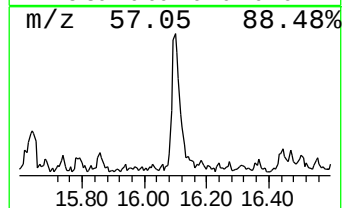
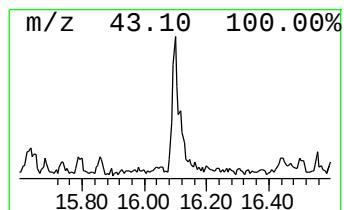
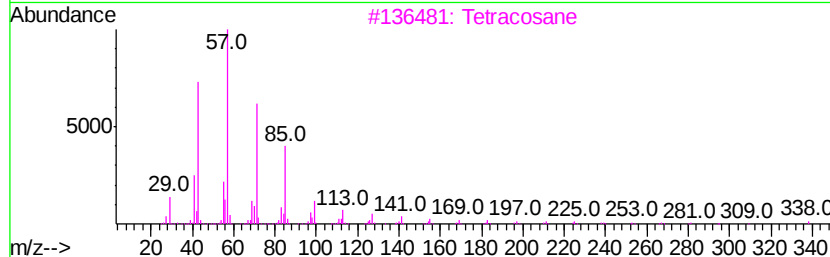
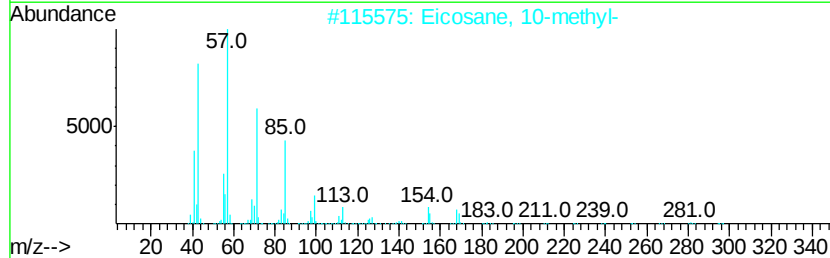
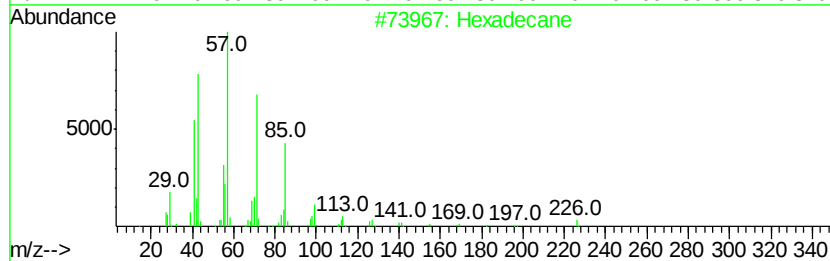
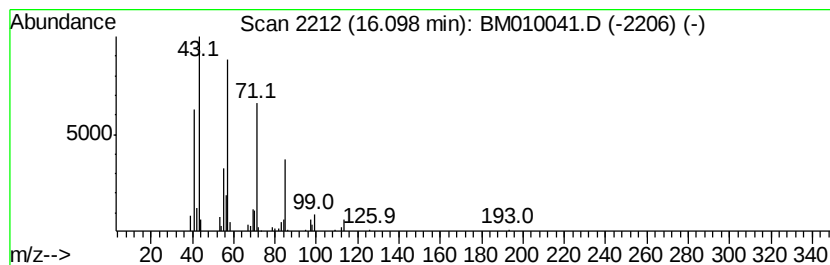
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.		
16.10	5.92 ng	212344	Phenanthrene-d10		17.17		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	91
2			Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
3			Tetracosane	338	C24H50	000646-31-1	90
4			Eicosane	282	C20H42	000112-95-8	90
5			Heptacosane	380	C27H56	000593-49-7	90



Data Path : Z:\HPCHEM1\BNA M\DATA\BM051517\
Data File : BM010041.D
Acq On : 15 May 2017 15:54
Operator : SJ/MA
Sample : I3100-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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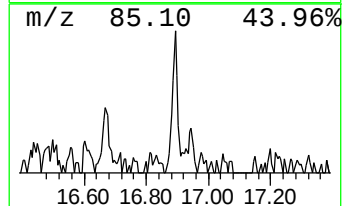
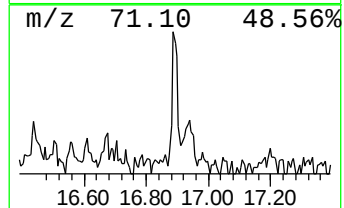
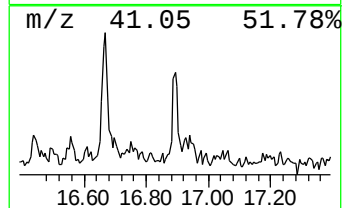
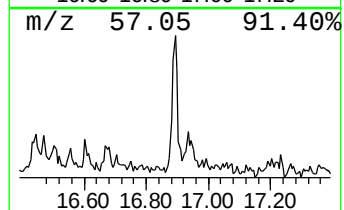
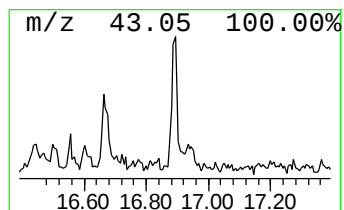
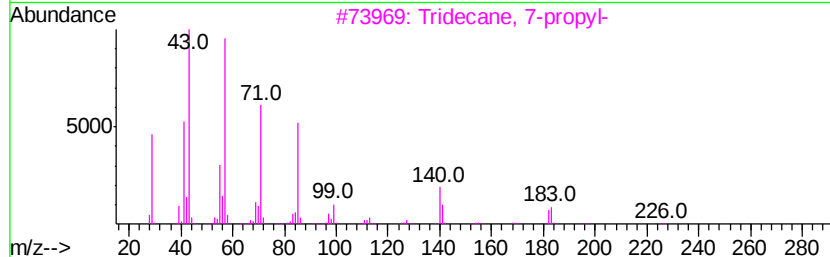
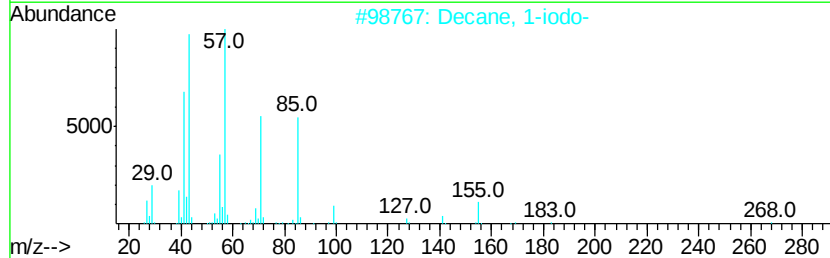
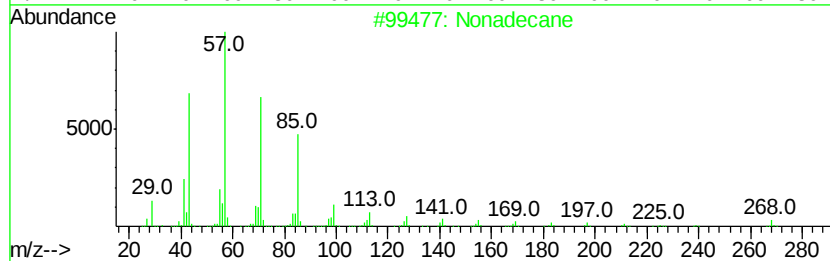
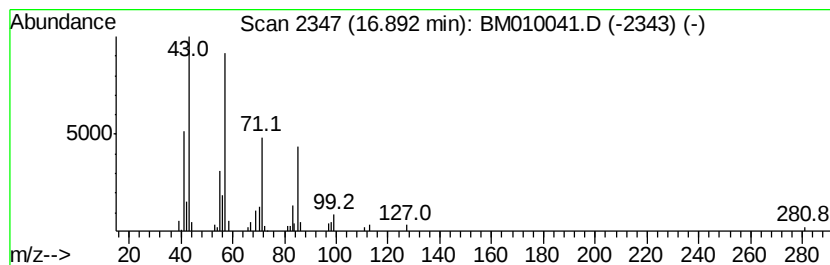
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Nonadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.89	2.12 ng	76256	Phenanthrene-d10	17.17

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	90
2			Decane, 1-iodo-	268	C10H21I	002050-77-3	83
3			Tridecane, 7-propyl-	226	C16H34	055045-09-5	80
4			Tridecane	184	C13H28	000629-50-5	78
5			1-Iodoundecane	282	C11H23I	004282-44-4	72



Data Path : Z:\HPCHEM1\BNA M\DATA\BM051517\
Data File : BM010041.D
Acq On : 15 May 2017 15:54
Operator : SJ/MA
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Misc :
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Instrument :
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ClientSampleId :
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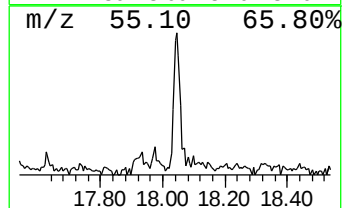
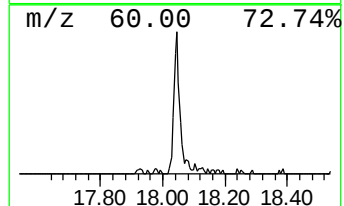
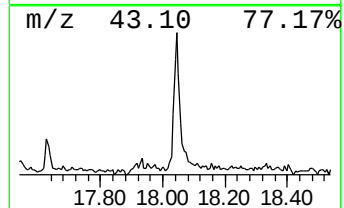
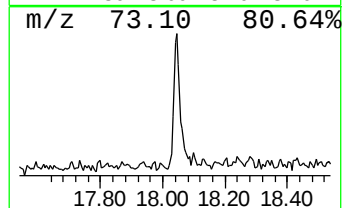
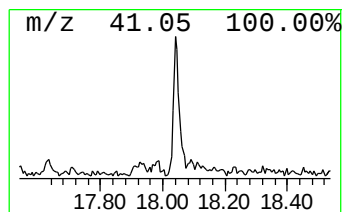
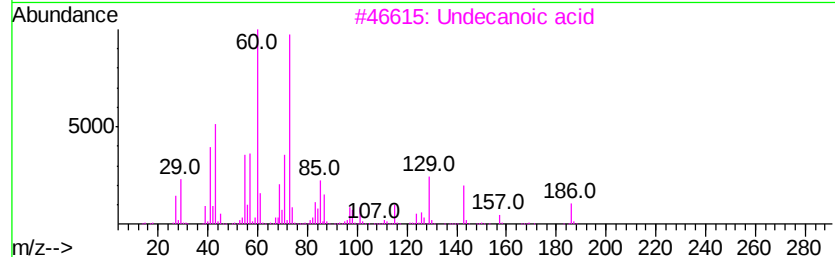
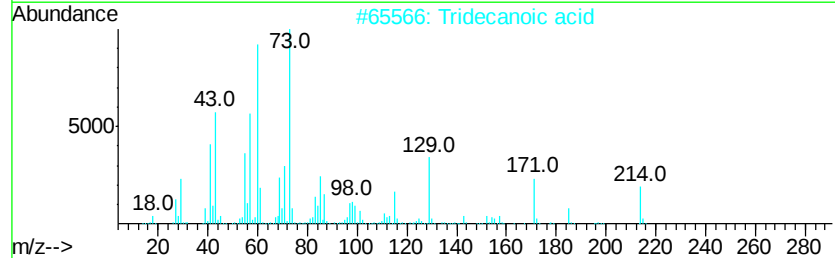
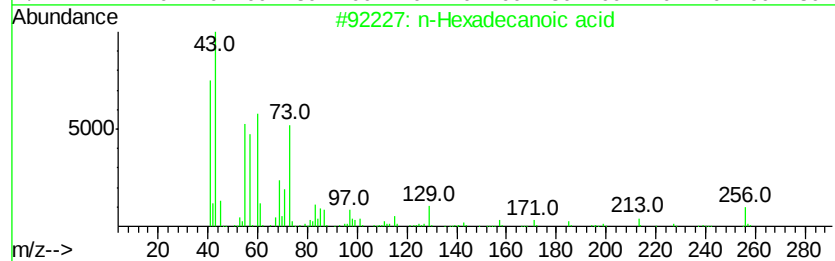
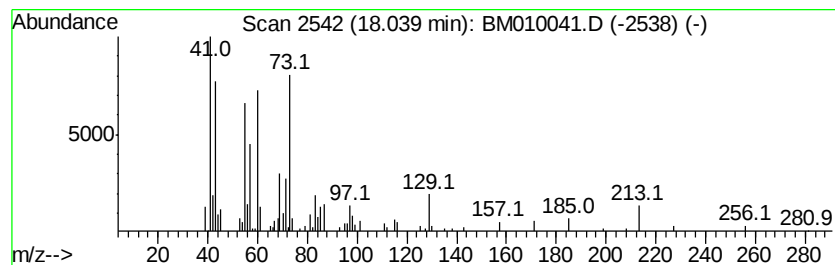
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.04	7.09 ng	254341	Phenanthrene-d10	17.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Undecanoic acid	186	C11H22O2	000112-37-8	72
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	59



Data Path : Z:\HPCHEM1\BNA M\DATA\BM051517\
Data File : BM010041.D
Acq On : 15 May 2017 15:54
Operator : SJ/MA
Sample : I3100-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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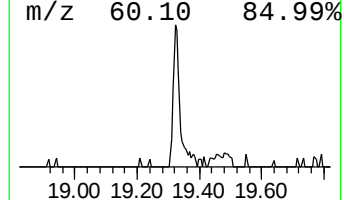
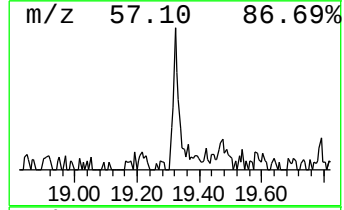
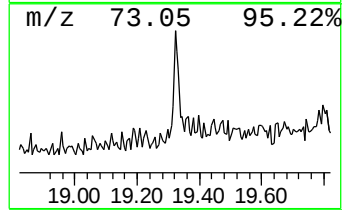
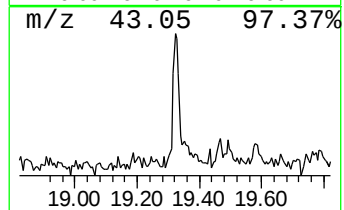
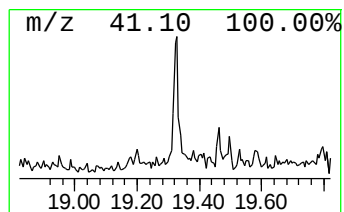
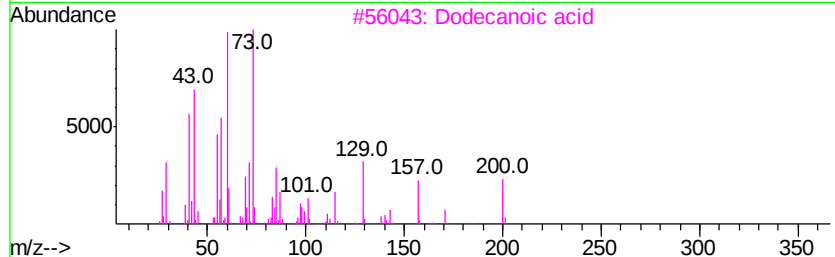
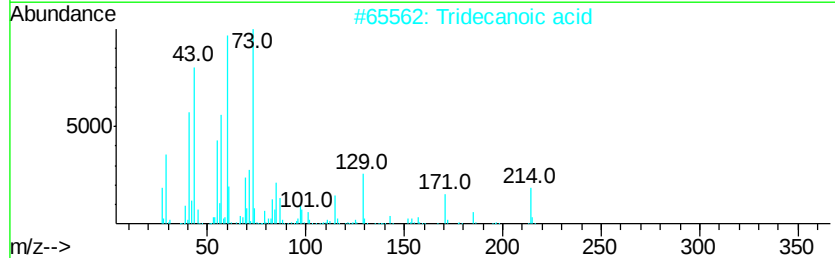
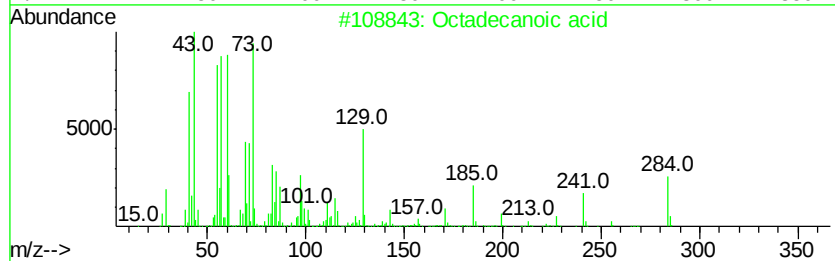
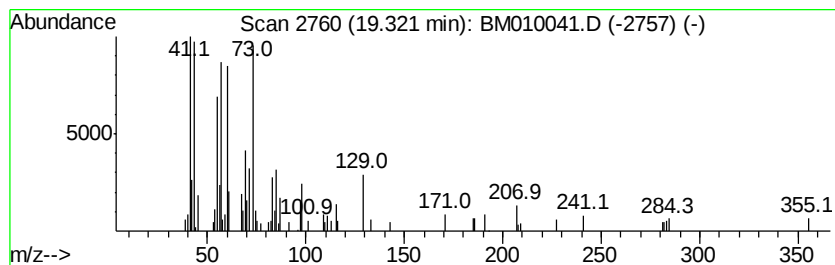
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.32	2.52 ng	118343	Chrysene-d12	21.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2		Tridecanoic acid	214	C13H26O2	000638-53-9	64
3		Dodecanoic acid	200	C12H24O2	000143-07-7	64
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	59
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	59



Data Path : Z:\HPCHEM1\BNA M\DATA\BM051517\
Data File : BM010041.D
Acq On : 15 May 2017 15:54
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Misc :
ALS Vial : 3 Sample Multiplier: 1

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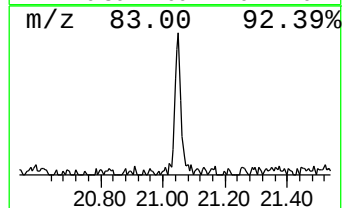
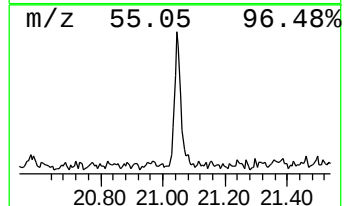
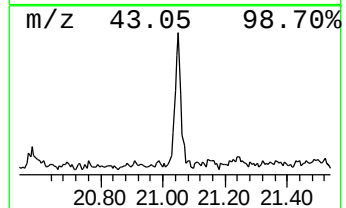
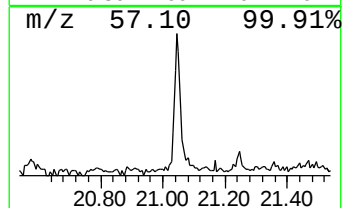
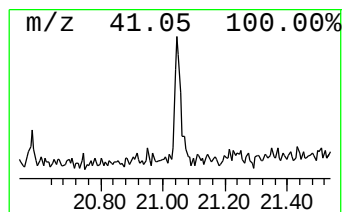
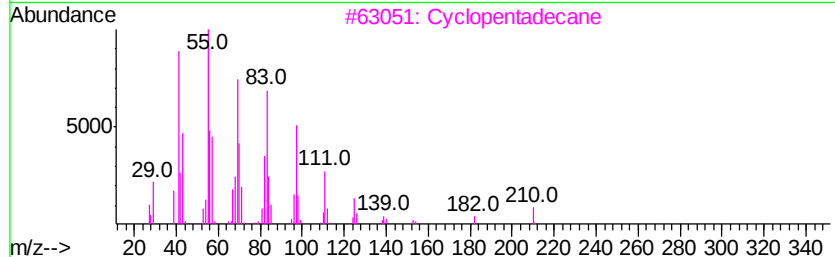
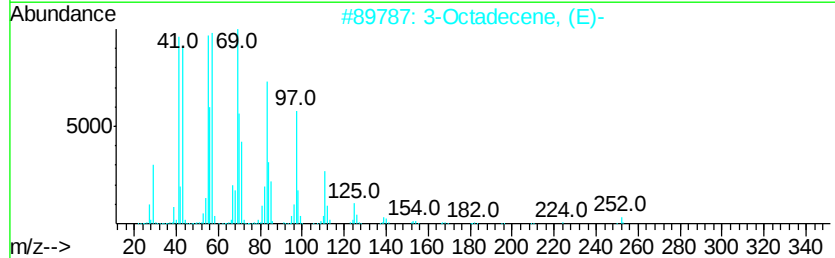
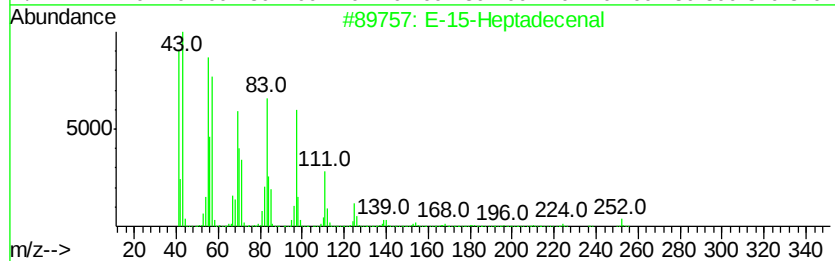
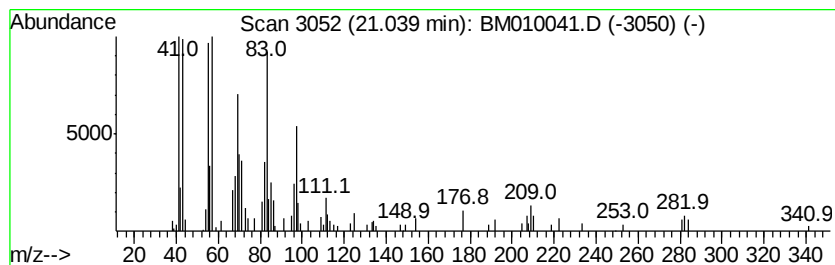
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 E-15-Heptadecenal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.04	4.07 ng	190942	Chrysene-d12	21.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	E-15-Heptadecenal	252	C17H32O	1000130-97-9	95
2		3-Octadecene, (E)-	252	C18H36	007206-19-1	92
3		Cyclopentadecane	210	C15H30	000295-48-7	91
4		1-Nonadecene	266	C19H38	018435-45-5	83
5		Cycloeicosane	280	C20H40	000296-56-0	83



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM051517\
Data File : BM010041.D
Acq On : 15 May 2017 15:54
Operator : SJ/MA
Sample : I3100-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PMW-2-051017

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown7.29	7.29	31.1	ng	729937	1	7.76	469554	20.0
unknown7.63	7.63	2.0	ng	47812	1	7.76	469554	20.0
Ethyl cyclopropan...	12.24	30.2	ng	854542	2	10.55	565148	20.0
Pentadecane	15.23	3.2	ng	102074	3	14.41	630453	20.0
1-Octanol, 2-butyl-	15.63	2.0	ng	63430	3	14.41	630453	20.0
Hexadecane	16.10	5.9	ng	212344	4	17.17	717722	20.0
Nonadecane	16.89	2.1	ng	76256	4	17.17	717722	20.0
n-Hexadecanoic acid	18.04	7.1	ng	254341	4	17.17	717722	20.0
Octadecanoic acid	19.32	2.5	ng	118343	5	21.36	939301	20.0
E-15-Heptadecenal	21.04	4.1	ng	190942	5	21.36	939301	20.0