

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF020419\
 Data File : BF112390.D
 Acq On : 4 Feb 2019 19:50
 Operator : JU/SJ
 Sample : K1360-01 2X
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RBR-200053

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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	5.040	499	502	515	rBV	58167	72593	4.25%	0.330%
2	5.463	570	574	591	rBV	1387887	1465746	85.72%	6.661%
3	6.081	676	679	683	rBV	103891	111459	6.52%	0.507%
4	6.475	742	746	762	rBV	1672440	1709948	100.00%	7.771%
5	6.604	764	768	778	rVV	2029734	1686471	98.63%	7.664%
6	6.828	803	806	815	rBV	1071598	934271	54.64%	4.246%
7	6.987	829	833	842	rBV	1268836	1140771	66.71%	5.184%
8	7.392	898	902	914	rBV	942437	983062	57.49%	4.468%
9	8.110	1020	1024	1032	rBV	1330326	1236178	72.29%	5.618%
10	9.186	1202	1207	1218	rBV	1612078	1512527	88.45%	6.874%
11	9.581	1271	1274	1280	rVB	177143	155511	9.09%	0.707%
12	9.869	1314	1323	1332	rBV	1571734	1449206	84.75%	6.586%
13	10.445	1418	1421	1423	rVB	47114	31827	1.86%	0.145%
14	10.657	1453	1457	1469	rBV	1187059	1114701	65.19%	5.066%
15	11.351	1572	1575	1578	rBV	1532685	1384458	80.96%	6.292%
16	11.375	1578	1579	1584	rVB	144150	104895	6.13%	0.477%
17	11.857	1659	1661	1662	rBV	24514	19532	1.14%	0.089%
18	11.874	1662	1664	1671	rVB4	105300	133610	7.81%	0.607%
19	11.969	1677	1680	1683	rBV2	25608	27945	1.63%	0.127%
20	12.404	1751	1754	1756	rBV	27150	23610	1.38%	0.107%
21	12.433	1756	1759	1762	rVV2	32427	28677	1.68%	0.130%
22	12.569	1778	1782	1787	rBV	185999	167799	9.81%	0.763%
23	12.657	1795	1797	1802	rBV3	40130	50048	2.93%	0.227%
24	12.798	1816	1821	1824	rBV	182958	204387	11.95%	0.929%
25	12.821	1824	1825	1828	rVB	42855	33815	1.98%	0.154%
26	12.933	1840	1844	1847	rBV	1458595	1244924	72.80%	5.658%
27	13.010	1854	1857	1865	rBV6	15147	27224	1.59%	0.124%
28	13.121	1870	1876	1879	rBV2	25751	53386	3.12%	0.243%
29	13.157	1879	1882	1886	rBV	68843	65654	3.84%	0.298%
30	13.233	1891	1895	1897	rVB3	21474	28592	1.67%	0.130%
31	13.498	1936	1940	1943	rBV2	116818	119946	7.01%	0.545%
32	13.639	1962	1964	1971	rVB6	19150	23221	1.36%	0.106%
33	13.827	1993	1996	1999	rBV	189624	168703	9.87%	0.767%
34	13.998	2020	2025	2028	rBV	1097314	1129854	66.08%	5.135%

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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 >
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.145	2047	2050	2053	rBV	280216	240435	14.06%	1.093%
36	14.451	2098	2102	2105	rBV	373094	356651	20.86%	1.621%
37	14.751	2149	2153	2157	rBV	420039	394455	23.07%	1.793%
38	15.086	2206	2210	2218	rVB	379802	475201	27.79%	2.160%
39	15.462	2269	2274	2280	rBV2	1070656	1386588	81.09%	6.302%
40	15.886	2342	2346	2351	rVB	221061	293736	17.18%	1.335%
41	16.380	2426	2430	2437	rVB2	125298	212156	12.41%	0.964%

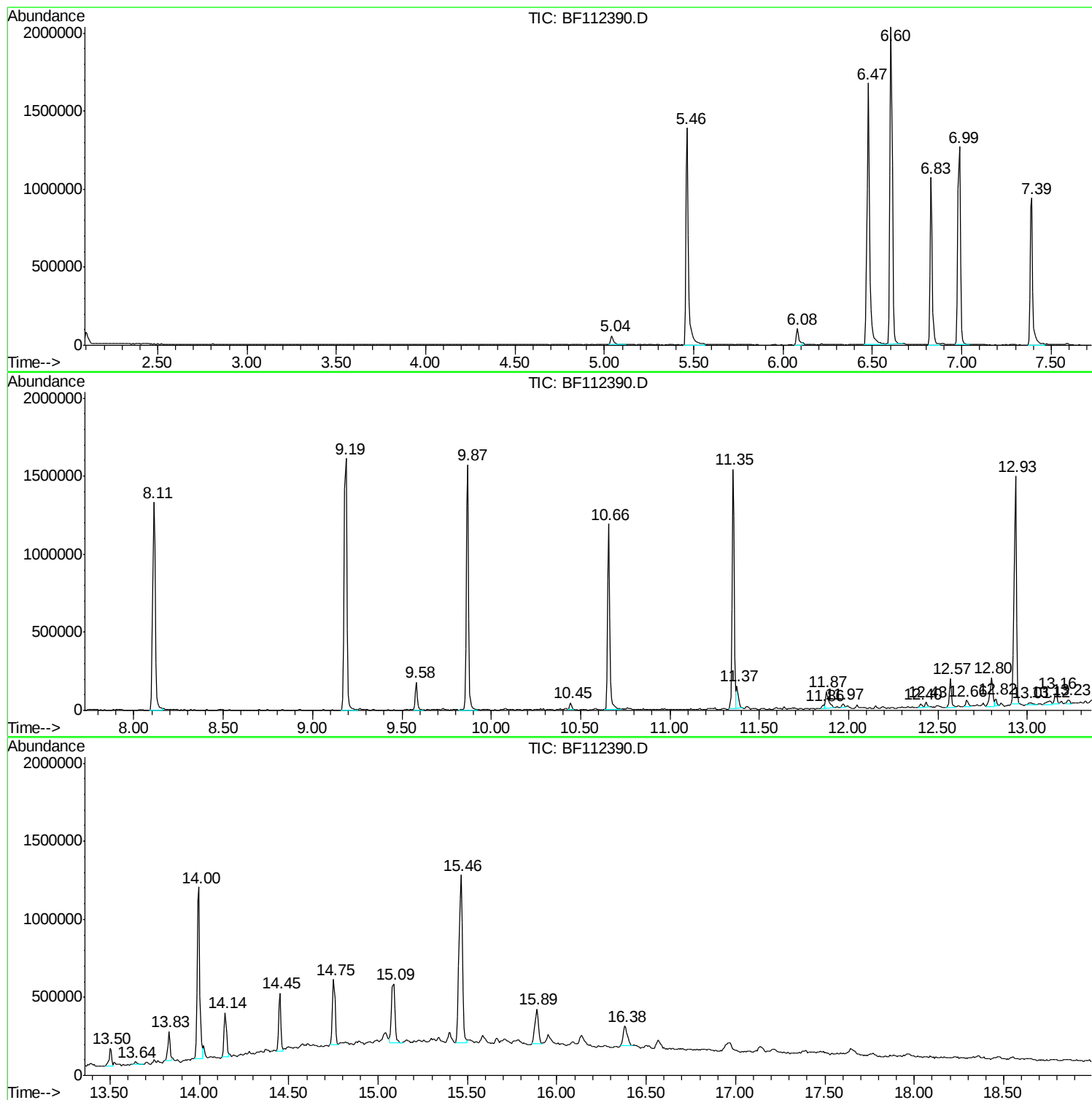
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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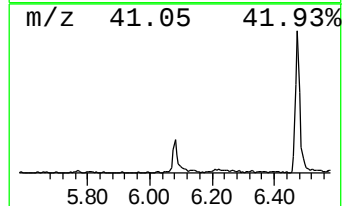
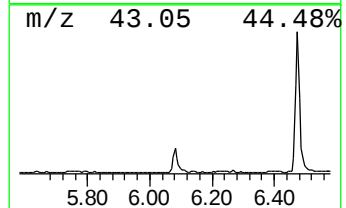
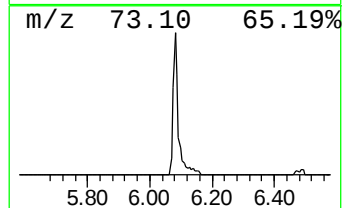
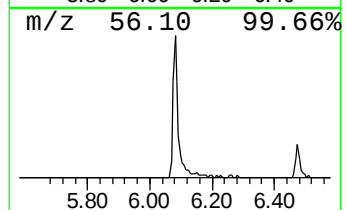
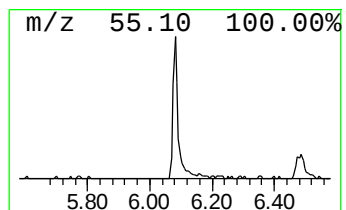
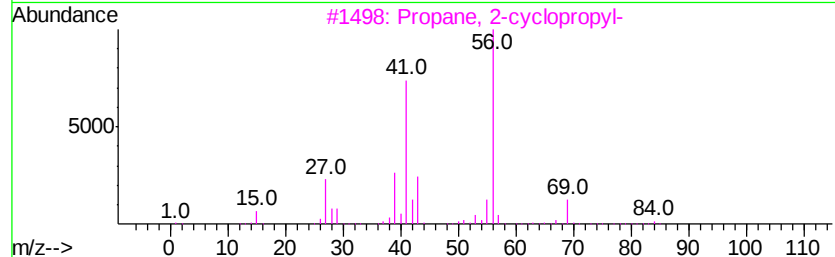
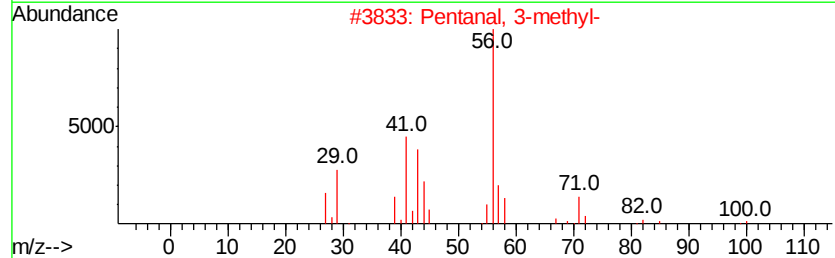
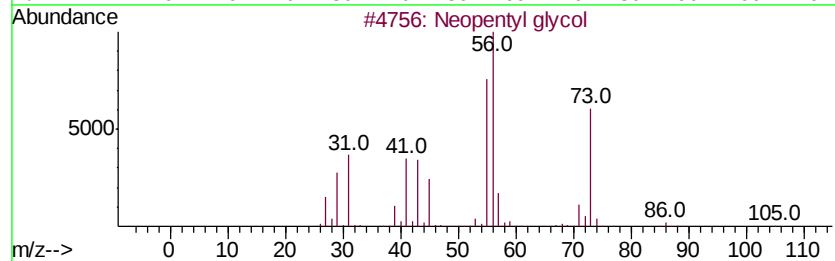
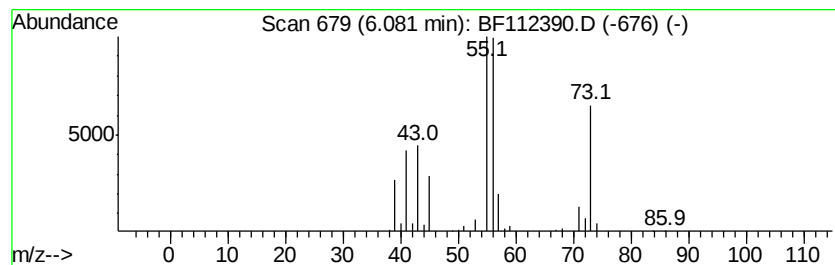
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Neopentyl glycol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.08	2.39 ng	111459	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Neopentyl glycol	104	C5H12O2	000126-30-7	83
2		Pentanal, 3-methyl-	100	C6H12O	015877-57-3	38
3		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	38
4		Oxirane, 2-methyl-3-(1-methylethyl)-	100	C6H12O	001192-31-0	33
5		Oxetane, 2,3,4-trimethyl-	100	C6H12O	053778-61-3	23



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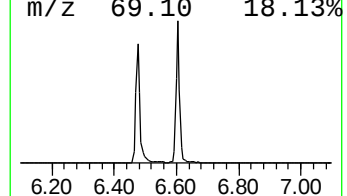
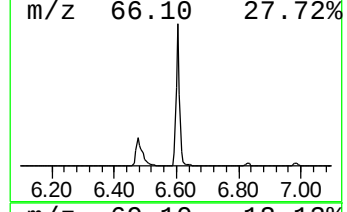
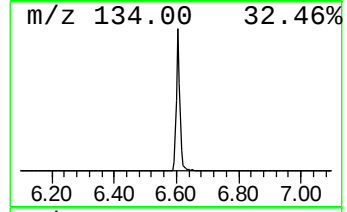
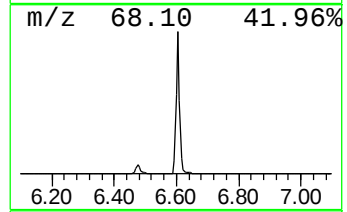
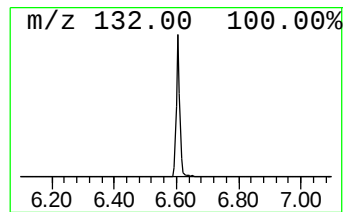
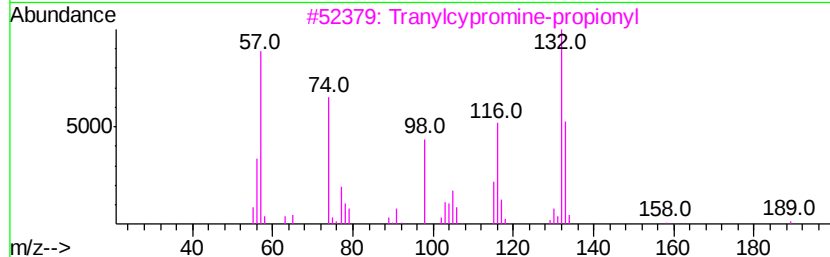
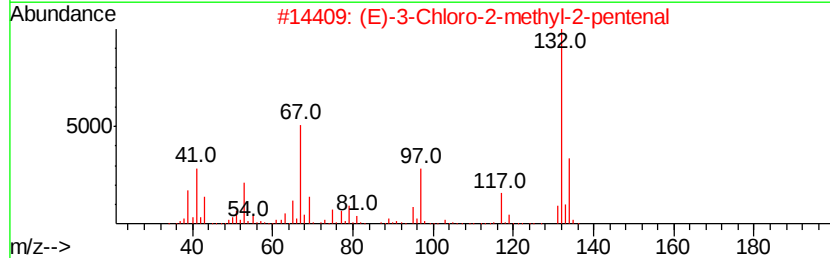
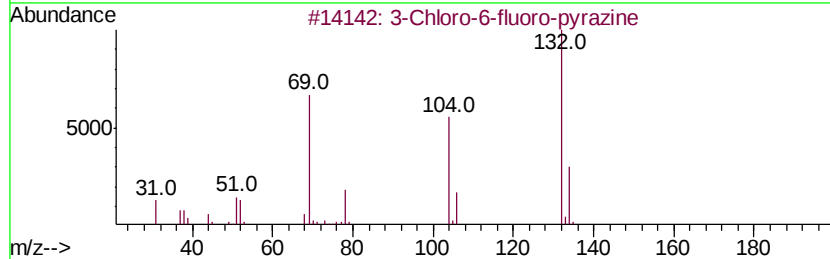
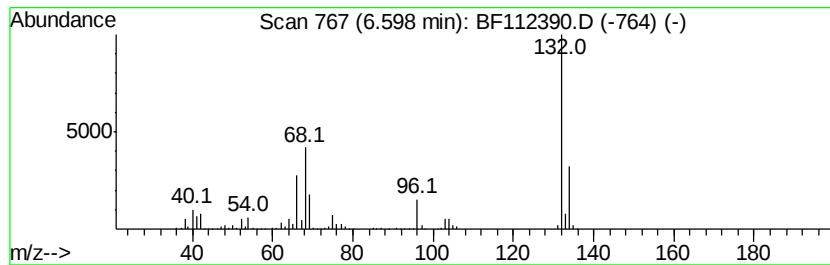
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Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	36.10 ng	1686470	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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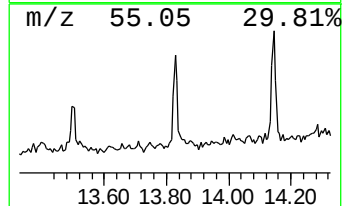
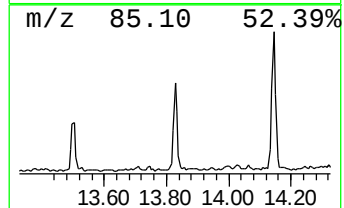
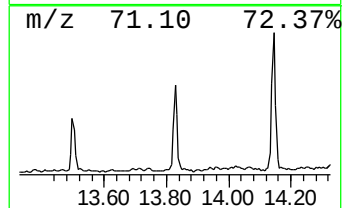
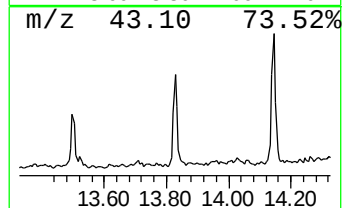
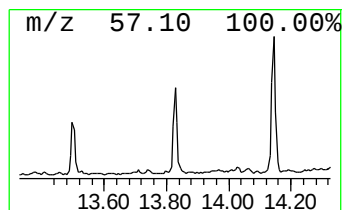
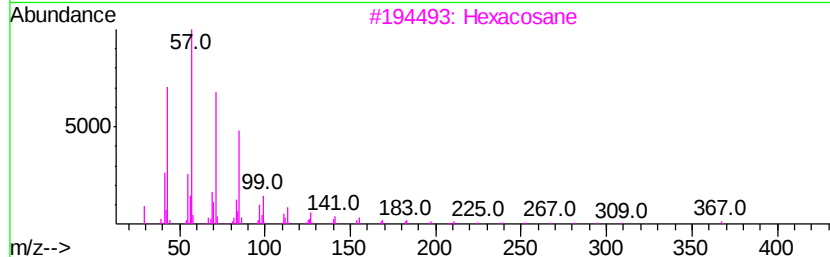
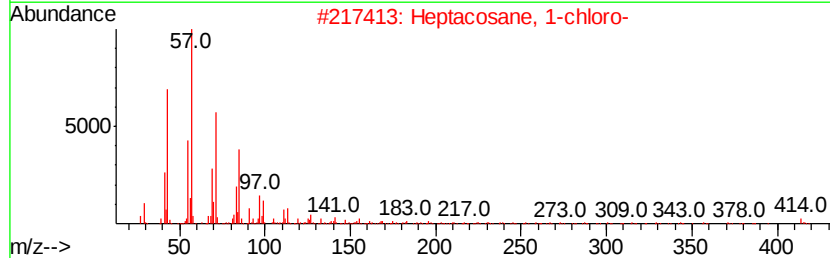
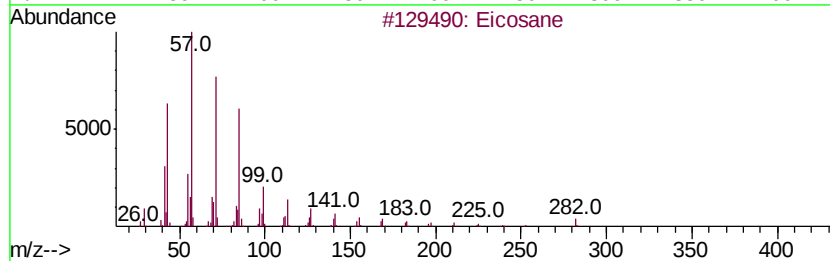
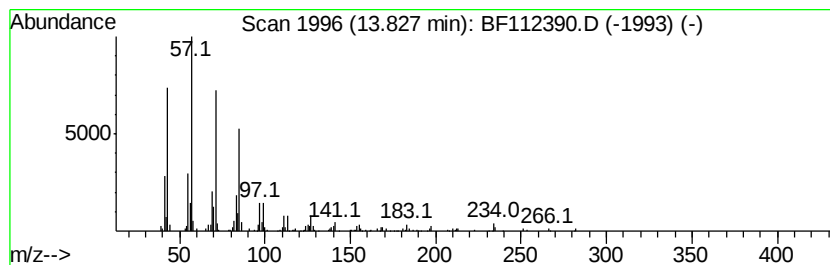
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	2.99 ng	168703	Chrysene-d12	14.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	90
2	Heptacosane, 1-chloro-		414	C27H55Cl	062016-79-9	90
3	Hexacosane		366	C26H54	000630-01-3	90
4	Heneicosane, 11-(1-ethylpropyl)-		366	C26H54	055282-11-6	87
5	10-Methylnonadecane		282	C20H42	056862-62-5	87



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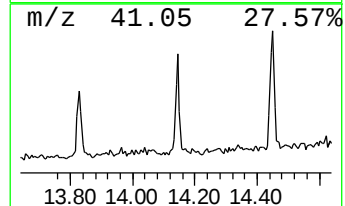
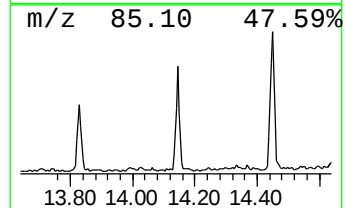
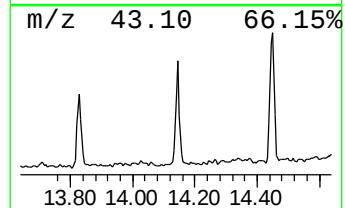
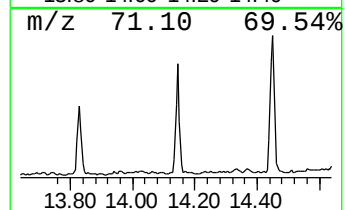
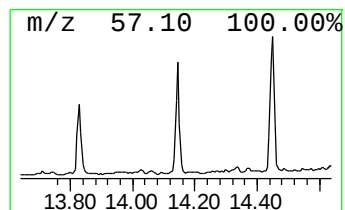
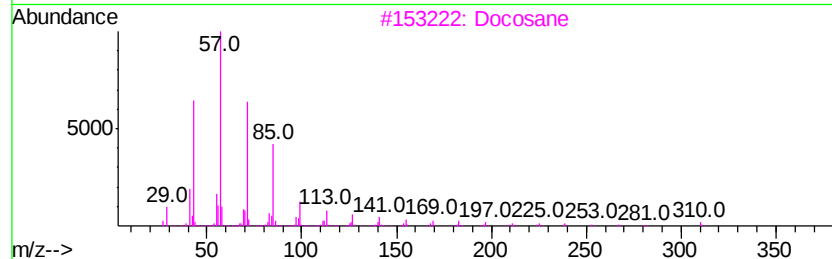
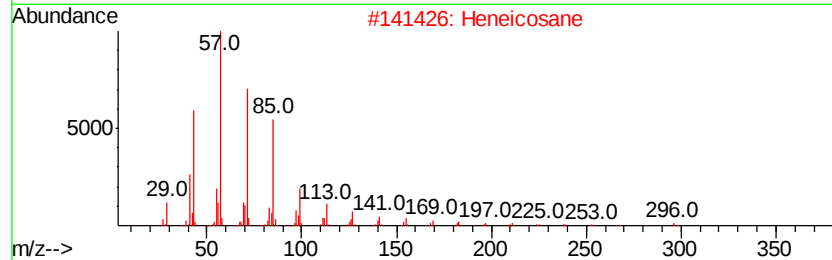
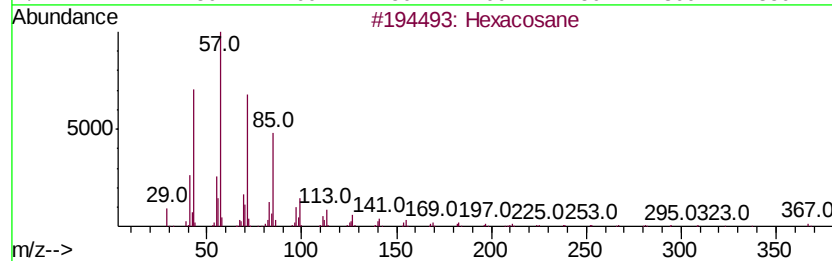
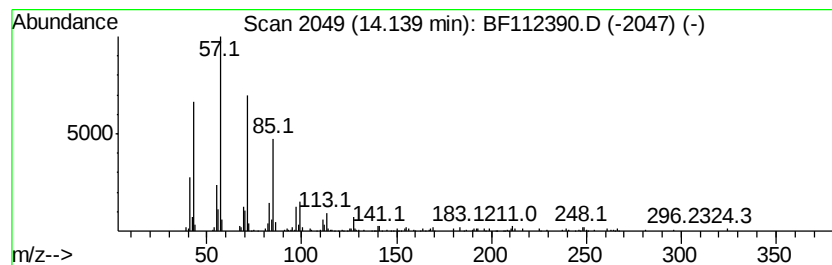
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.14	4.26 ng	240435	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	90
2		Heneicosane	296	C21H44	000629-94-7	90
3		Docosane	310	C22H46	000629-97-0	87
4		Heptadecane	240	C17H36	000629-78-7	87
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87



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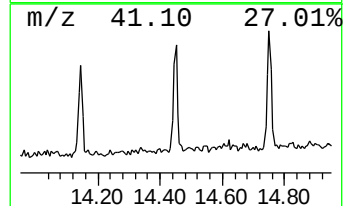
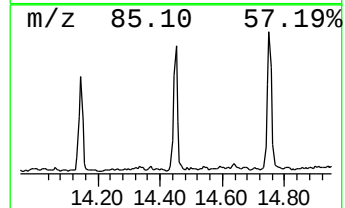
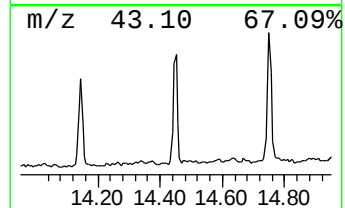
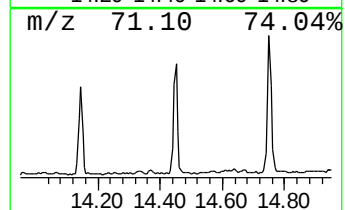
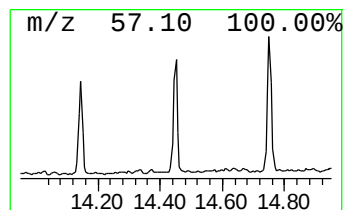
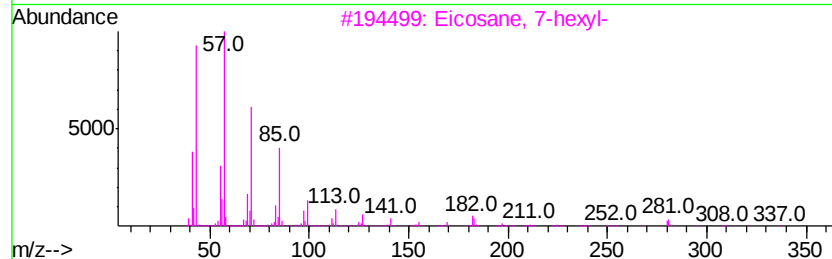
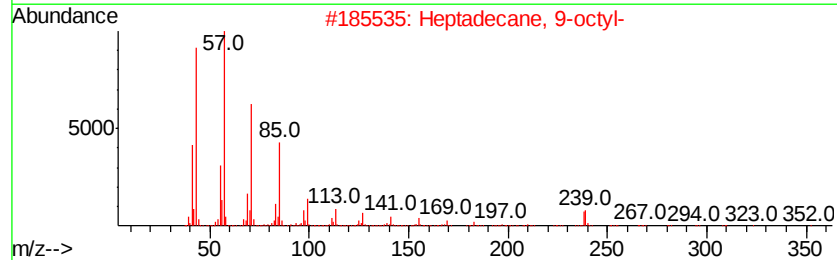
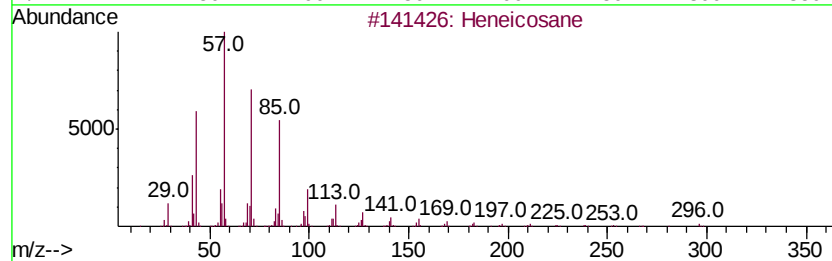
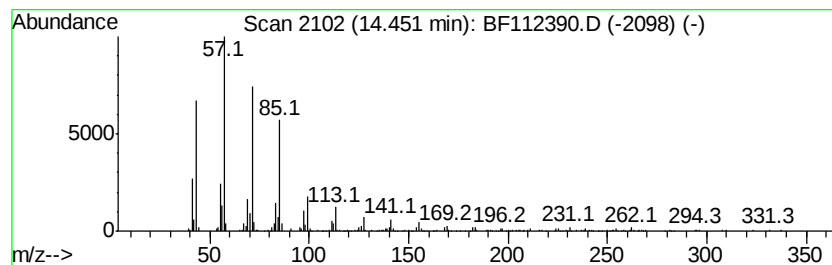
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Peak Number 7 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	6.31 ng	356651	Chrysene-d12	14.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	95
2	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
3	Eicosane, 7-hexyl-		366	C26H54	055333-99-8	91
4	Docosane, 11-butyl-		366	C26H54	013475-76-8	91
5	Heptadecane		240	C17H36	000629-78-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020419\
Data File : BF112390.D
Acq On : 4 Feb 2019 19:50
Operator : JU/SJ
Sample : K1360-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-200053

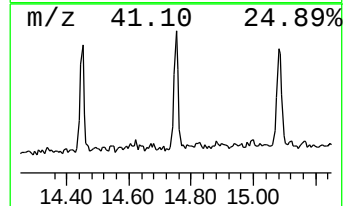
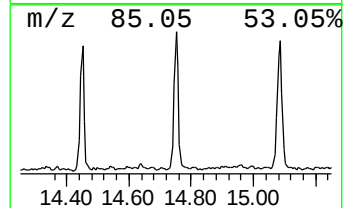
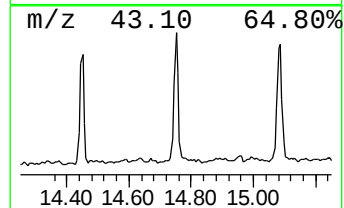
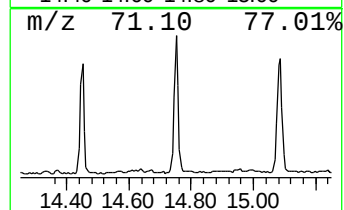
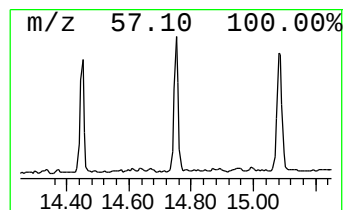
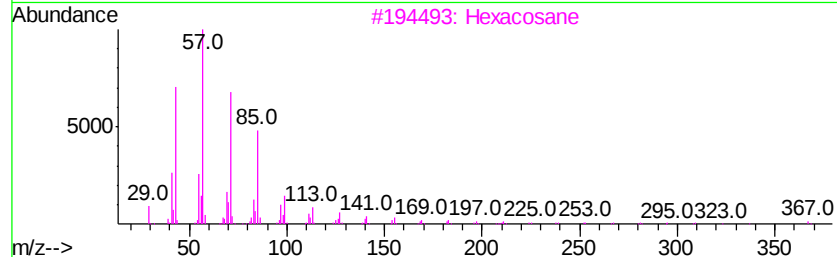
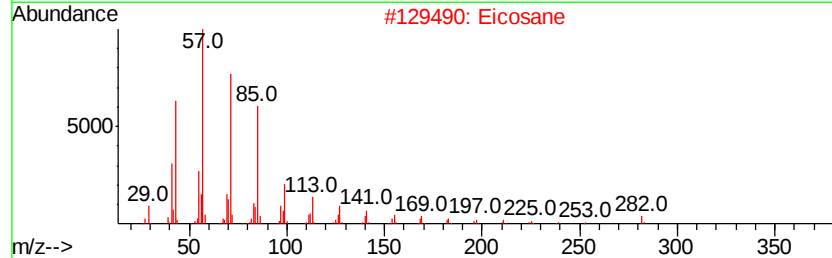
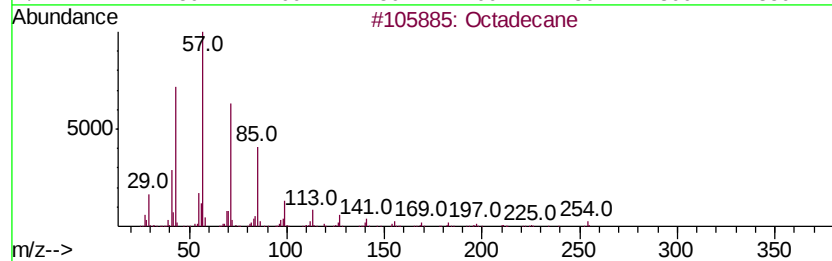
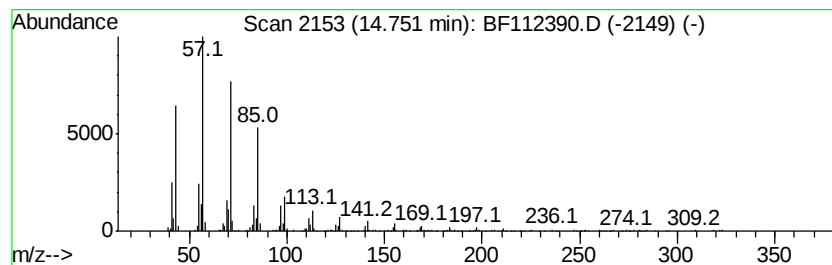
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	5.69 ng	394455	Perylene-d12	15.46

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane		254	C18H38	000593-45-3	95
2	Eicosane		282	C20H42	000112-95-8	95
3	Hexacosane		366	C26H54	000630-01-3	91
4	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
5	Heneicosane		296	C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020419\
Data File : BF112390.D
Acq On : 4 Feb 2019 19:50
Operator : JU/SJ
Sample : K1360-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-200053

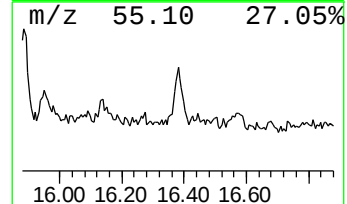
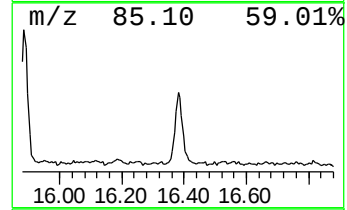
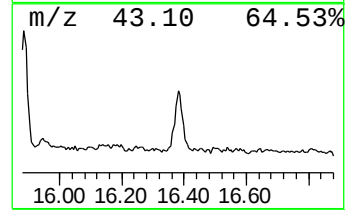
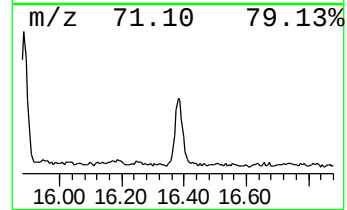
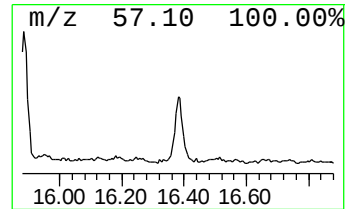
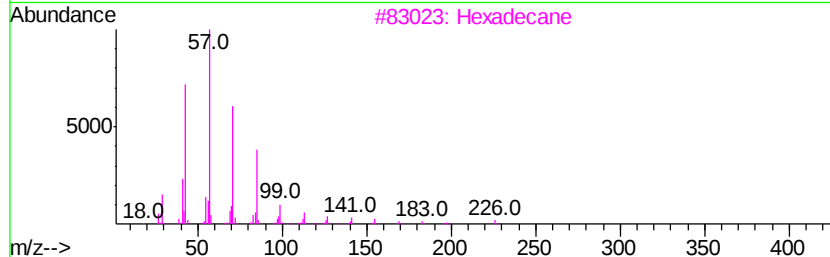
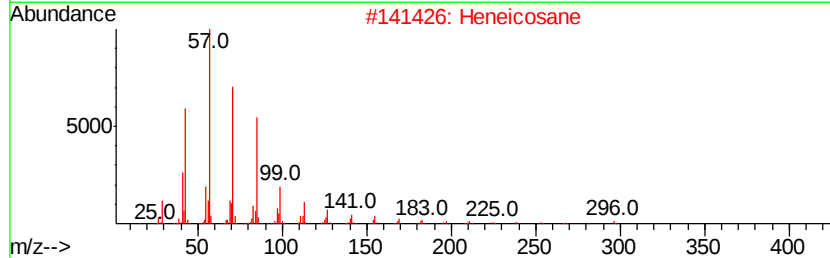
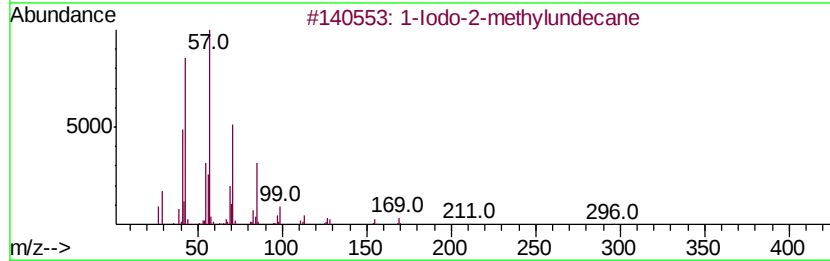
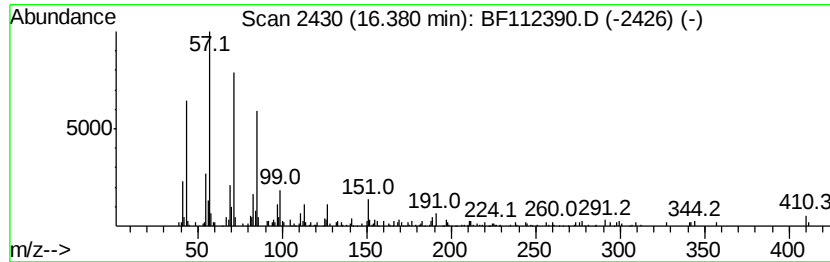
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Iodo-2-methylundecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.38	3.06 ng	212156	Perylene-d12	15.46

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	90
2			Heneicosane	296	C21H44	000629-94-7	87
3			Hexadecane	226	C16H34	000544-76-3	87
4			Tridecane, 6-propyl-	226	C16H34	055045-10-8	87
5			Hexacosane	366	C26H54	000630-01-3	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF020419\
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Acq On : 4 Feb 2019 19:50
Operator : JU/SJ
Sample : K1360-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-200053

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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
Neopentyl glycol	6.08	2.4	ng	111459	1	6.83	934271	20.0
unknown6.60	6.60	36.1	ng	1686470	1	6.83	934271	20.0
Eicosane	13.83	3.0	ng	168703	5	14.00	1129850	20.0
Hexacosane	14.14	4.3	ng	240435	5	14.00	1129850	20.0
Heneicosane	14.45	6.3	ng	356651	5	14.00	1129850	20.0
Octadecane	14.75	5.7	ng	394455	6	15.46	1386590	20.0
1-Iodo-2-methylun...	16.38	3.1	ng	212156	6	15.46	1386590	20.0