

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF011720\
 Data File : BF118575.D
 Acq On : 17 Jan 2020 23:14
 Operator : JU
 Sample : PB126175BL
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB126175BL

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011720.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	2.169	7	14	20	rVB	6598593	9366757	64.11%	10.529%
2	5.093	505	511	518	rVB	203164	230940	1.58%	0.260%
3	5.499	575	580	583	rBV	4173011	3635154	24.88%	4.086%
4	6.498	746	750	753	rBV	2858023	2324467	15.91%	2.613%
5	6.651	772	776	780	rBV	7041769	6860387	46.96%	7.712%
6	6.887	812	816	820	rBV	2583022	2070255	14.17%	2.327%
7	7.046	839	843	846	rBV	9095543	7919103	54.20%	8.902%
8	7.445	906	911	914	rBV	6674232	6372819	43.62%	7.163%
9	8.169	1030	1034	1037	rBV	3160750	2576349	17.63%	2.896%
10	8.704	1115	1125	1138	rVB	261008	401965	2.75%	0.452%
11	9.245	1212	1217	1220	rBV	12394355	12019788	82.27%	13.511%
12	9.628	1272	1282	1287	rBV	324248	379978	2.60%	0.427%
13	9.922	1328	1332	1336	rBV	3590688	3096706	21.20%	3.481%
14	10.710	1461	1466	1469	rBV	6173239	5484529	37.54%	6.165%
15	11.410	1580	1585	1588	rBV	3485011	3263816	22.34%	3.669%
16	12.998	1850	1855	1858	rBV	14007983	14610294	100.00%	16.423%
17	14.045	2029	2033	2036	rBV	3528728	3225659	22.08%	3.626%
18	14.522	2111	2114	2117	rVB	274759	223832	1.53%	0.252%
19	14.833	2163	2167	2175	rBV	382790	389870	2.67%	0.438%
20	15.174	2221	2225	2231	rBV	401186	428221	2.93%	0.481%
21	15.516	2277	2283	2288	rBV	2504306	3039527	20.80%	3.417%
22	15.563	2288	2291	2298	rVB	368005	453877	3.11%	0.510%
23	16.010	2362	2367	2379	rBV	231410	365421	2.50%	0.411%
24	16.527	2450	2455	2464	rVB	119977	223064	1.53%	0.251%

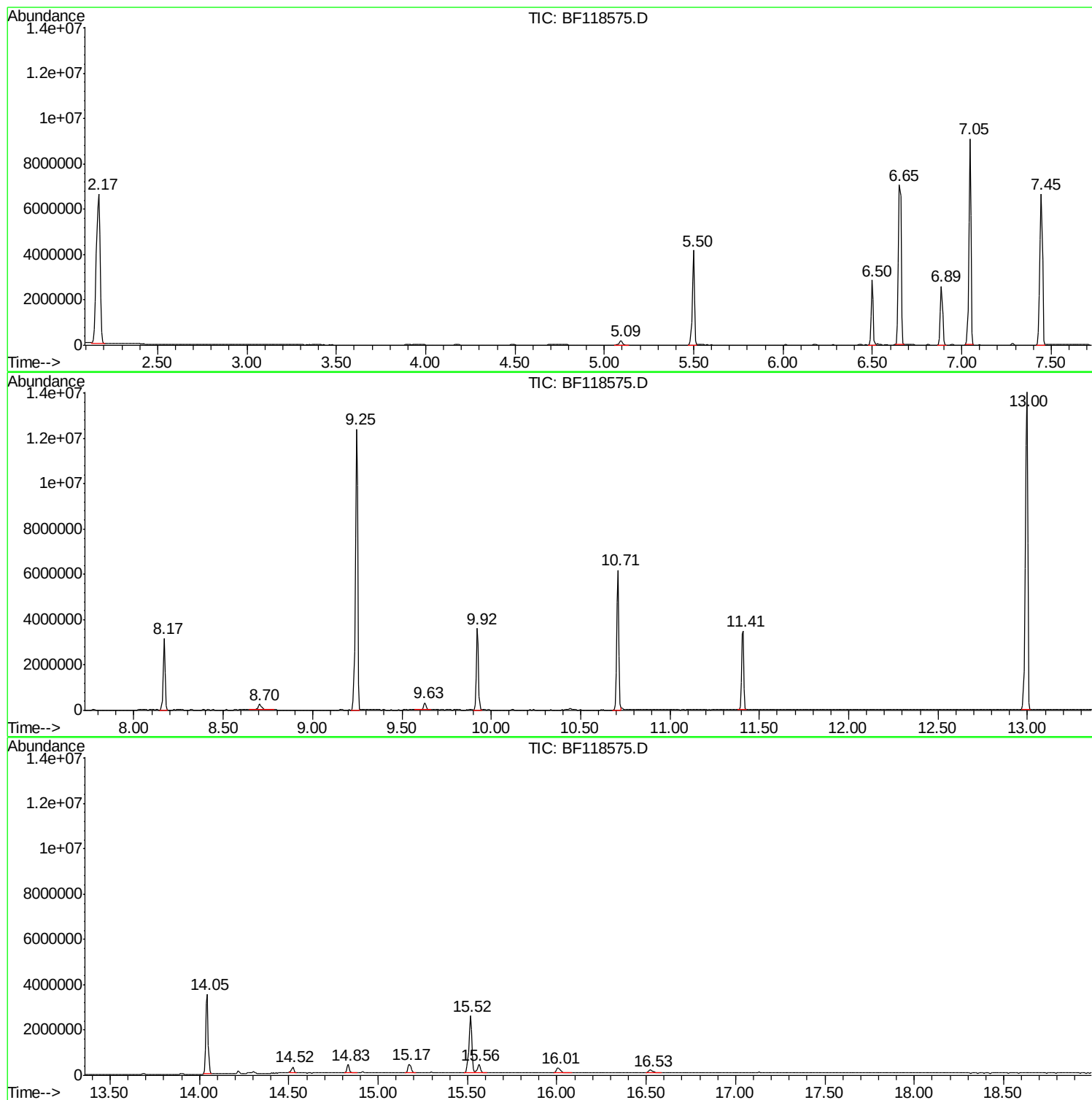
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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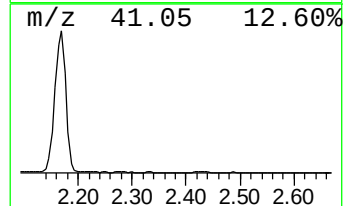
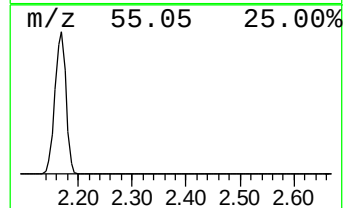
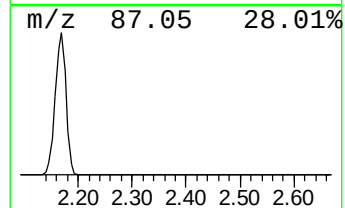
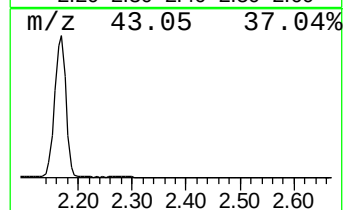
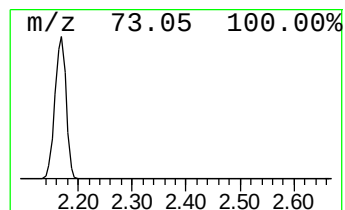
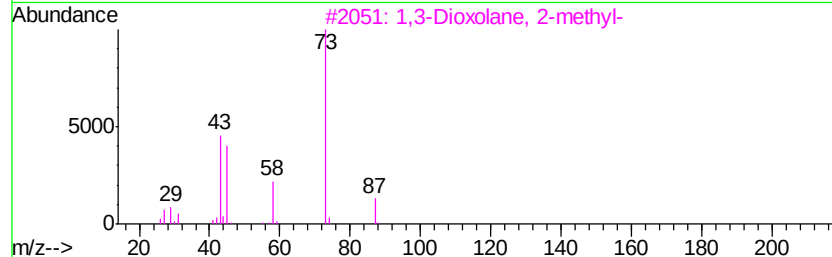
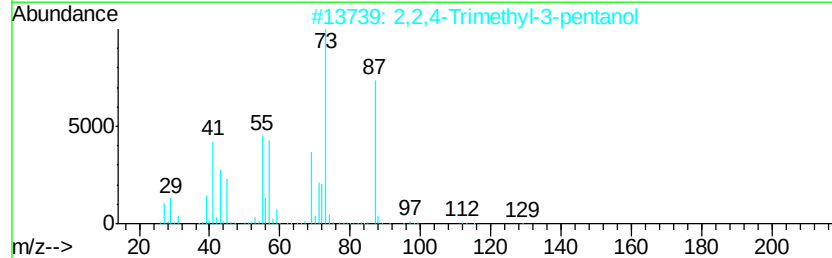
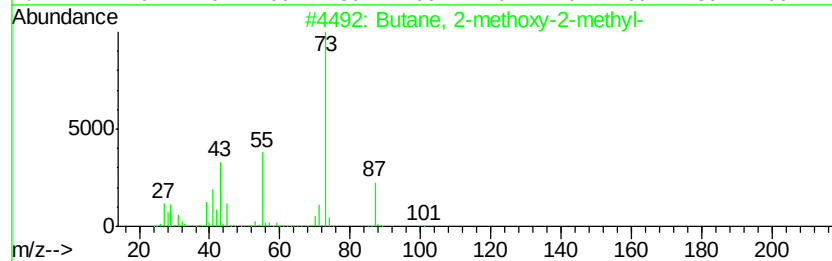
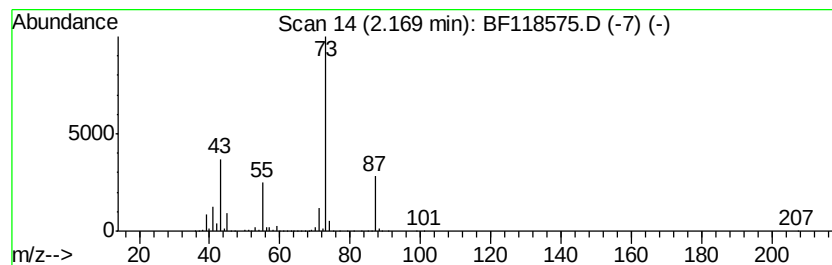
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF011720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	90.49 ng	9366760	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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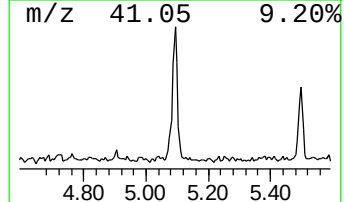
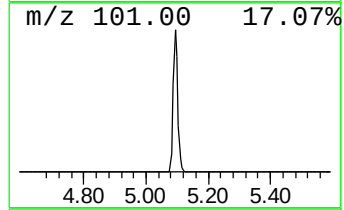
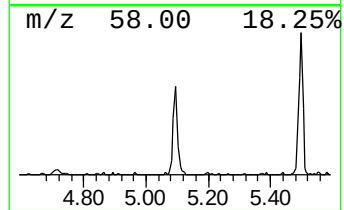
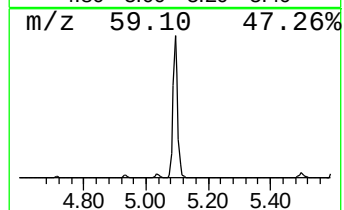
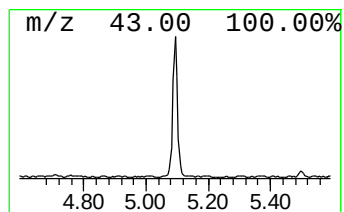
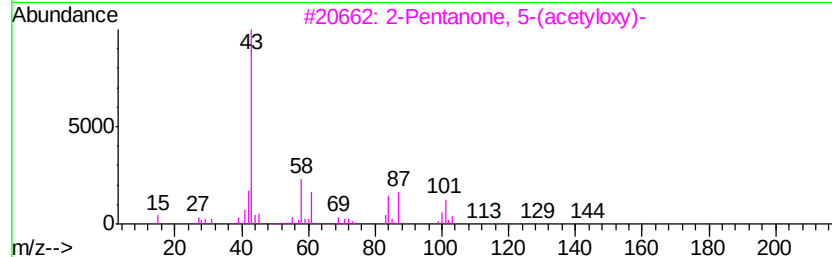
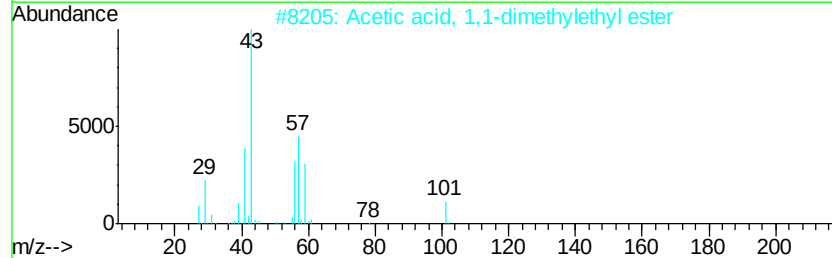
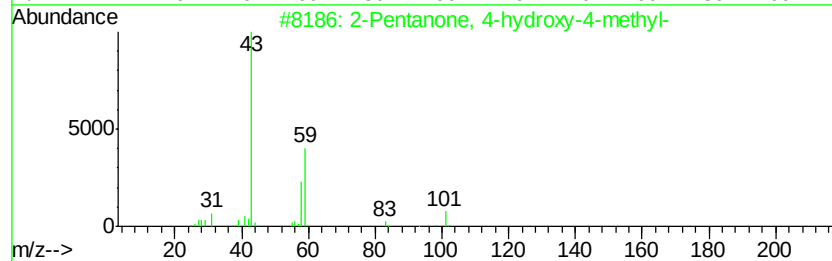
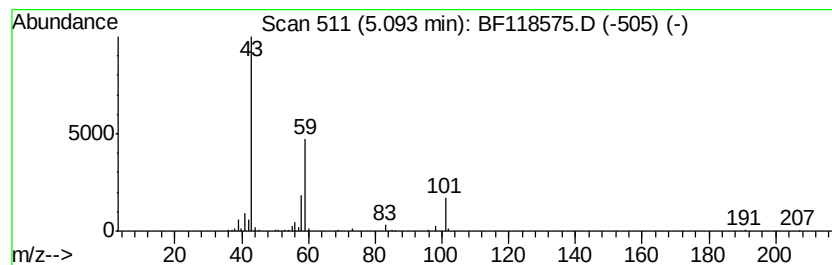
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	2.23 ng	230940	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3		2-Pentanone, 5-(acetyloxy)-	144	C7H12O3	005185-97-7	17
4		Acetone	58	C3H6O	000067-64-1	14
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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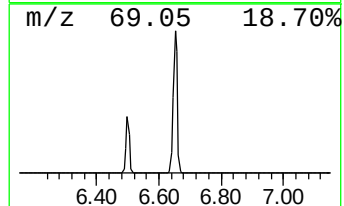
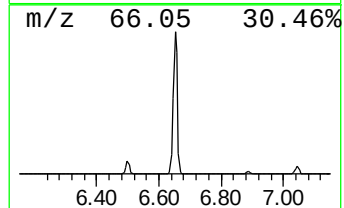
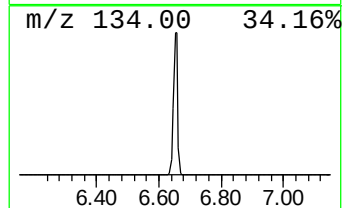
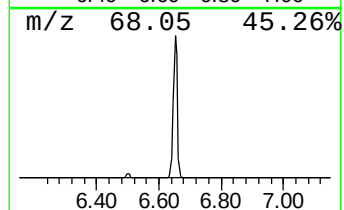
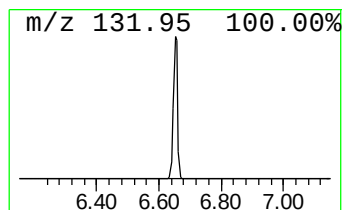
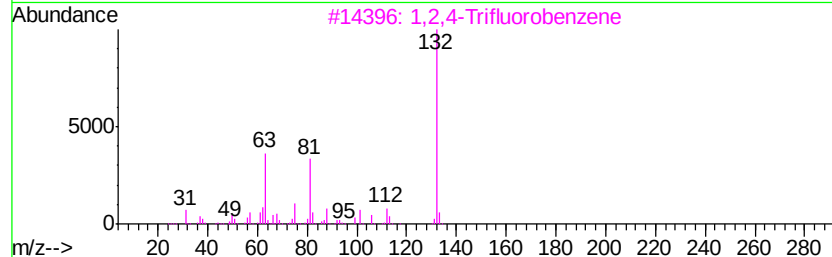
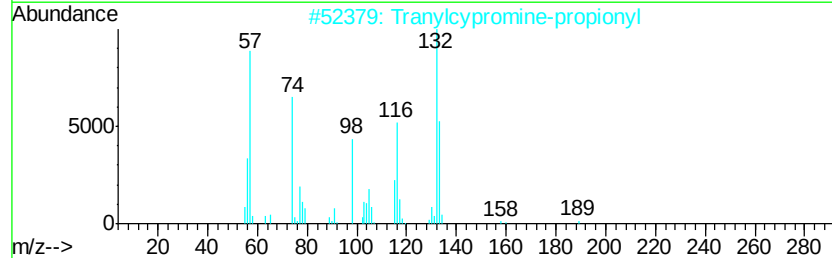
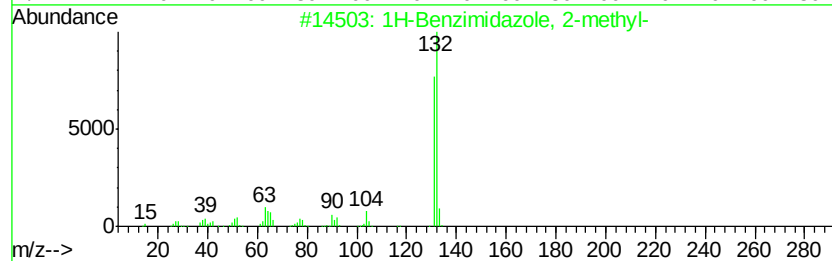
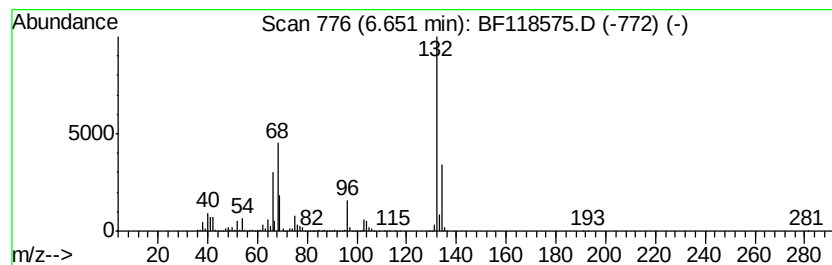
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Peak Number 3 unknown6.65 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	66.28 ng	6860390	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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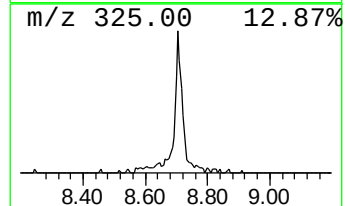
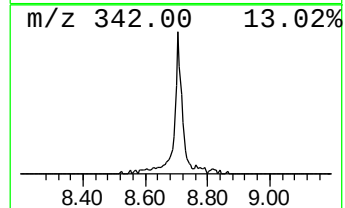
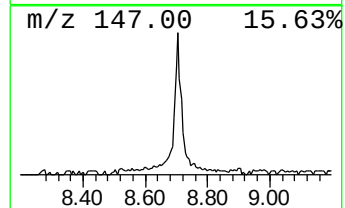
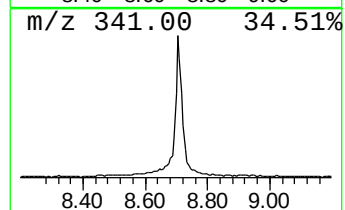
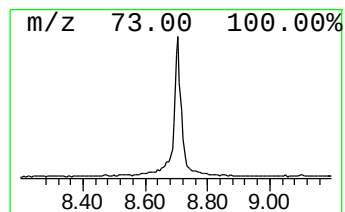
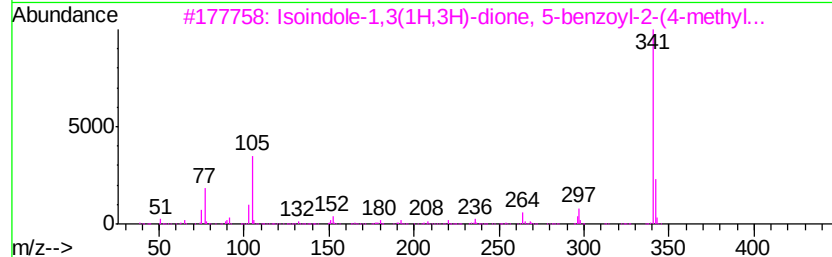
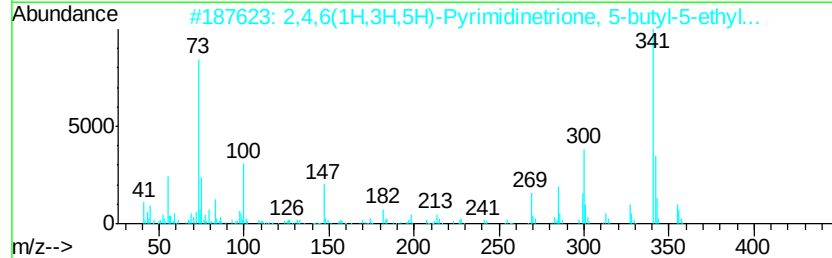
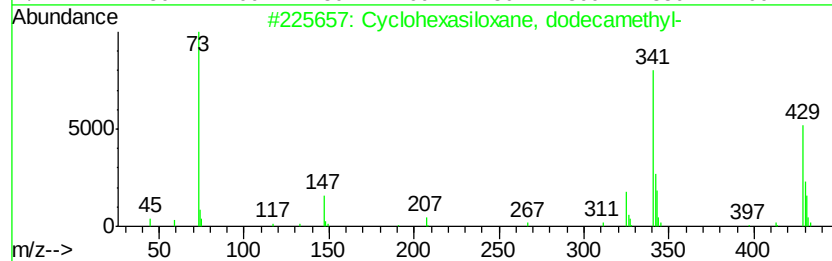
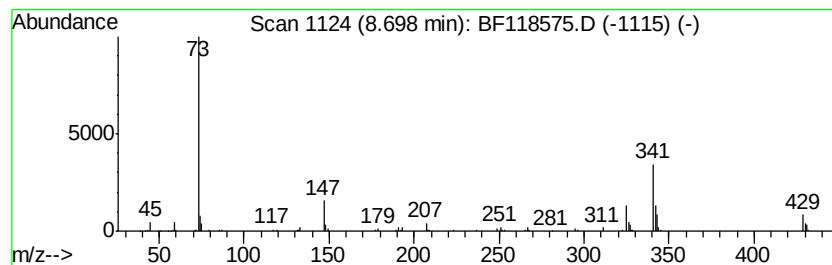
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Peak Number 5 Cyclohexasiloxane, dodecane... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.70	3.12 ng	401965	Naphthalene-d8	8.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexasiloxane, dodecamethyl-	444	C12H36O6Si6	000540-97-6	91
2		2,4,6(1H,3H,5H)-Pyrimidinetrione...	356	C16H32N2O3Si2	052988-92-8	36
3		Isoindole-1,3(1H,3H)-dione, 5-be...	341	C22H15N03	331269-95-5	35
4		Acetic acid, [bis[(trimethylsilyl...	356	C11H29O5PSi3	053044-27-2	33
5		2H-1,4-Benzodiazepin-2-one, 7-ch...	342	C18H19ClN2OSi	055299-24-6	25



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TIC Integration Parameters: LSCINT.P

Peak Number 6 Cycloheptasiloxane, tetradec... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
9.63	2.45 ng	379978	Acenaphthene-d10	9.92		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cycloheptasiloxane, tetradecamethyl-	518	C14H42O7Si7	000107-50-6	90
2		2',6'-Dihydroxyacetophenone, bis(trimethylsilyl) ...	296	C14H24O3Si2	1000352-81-3	42
3		Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	38
4		Trisiloxane, 1,1,1,5,5,5-hexamethyl-	384	C12H36O4Si5	003555-47-3	38
5		Hexasiloxane, 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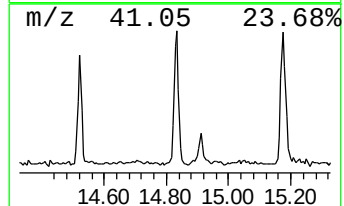
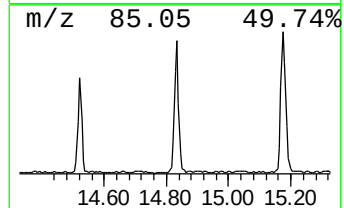
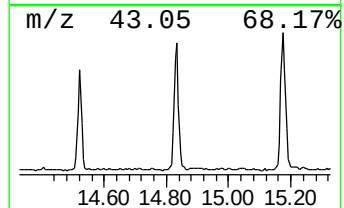
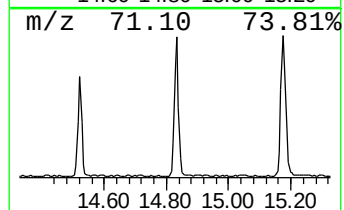
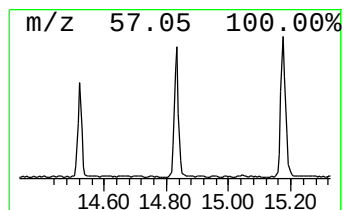
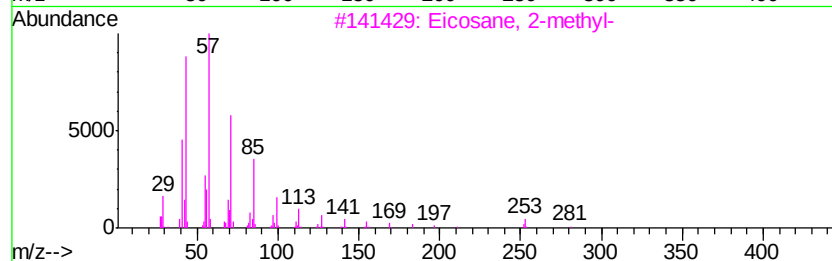
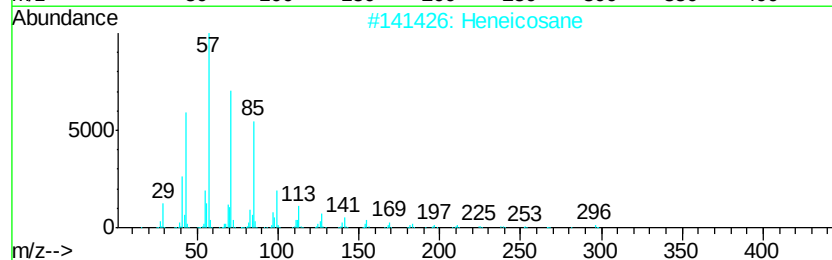
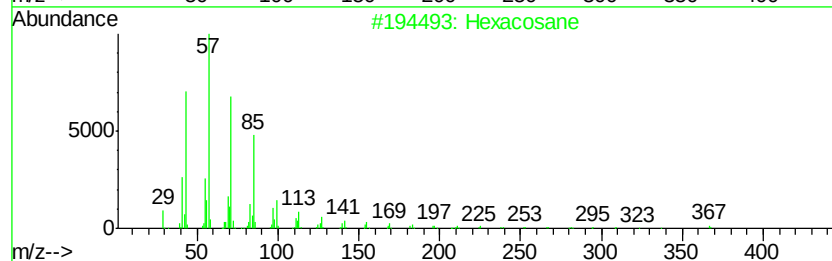
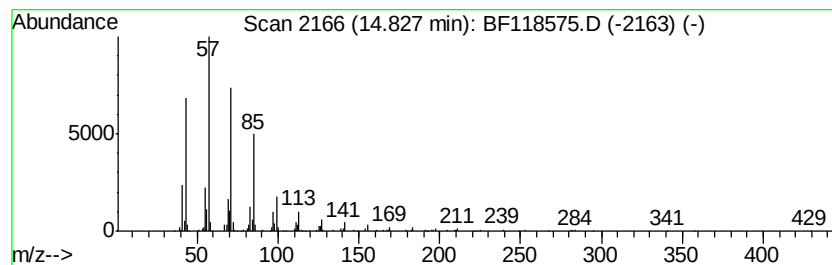
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Peak Number 7 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	2.57 ng	389870	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Eicosane, 2-methyl-	296	C21H44	001560-84-5	91
4		Tetracosane	338	C24H50	000646-31-1	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011720\
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Acq On : 17 Jan 2020 23:14
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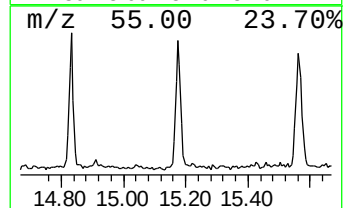
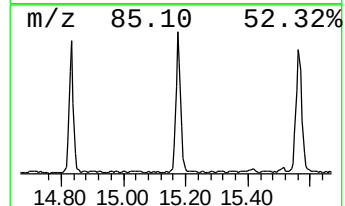
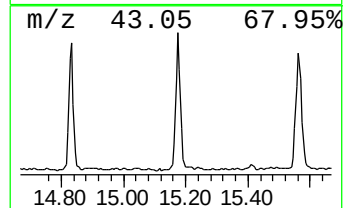
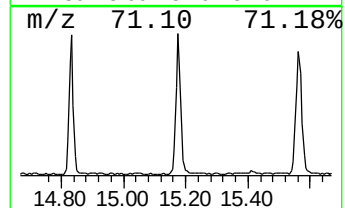
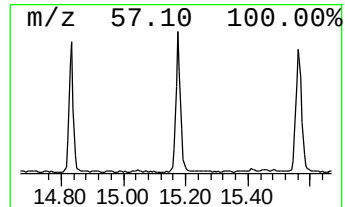
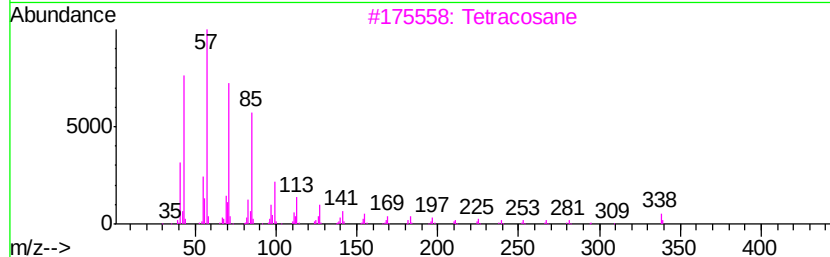
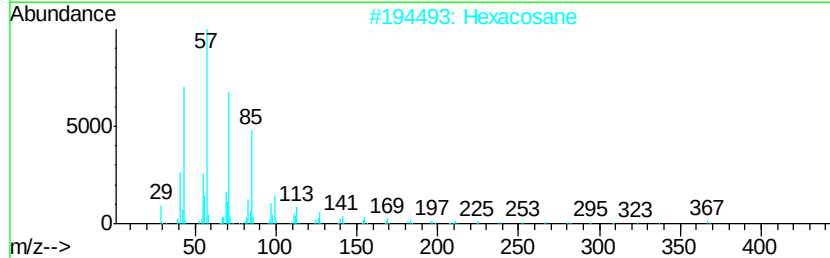
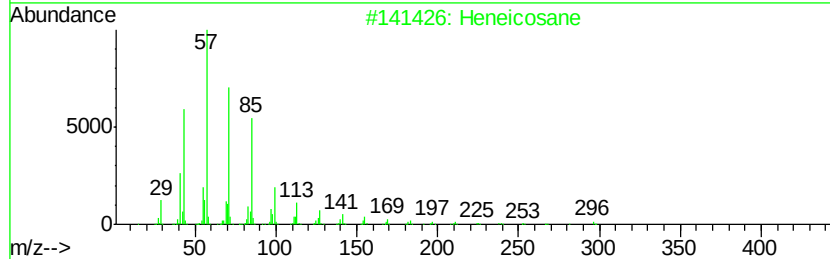
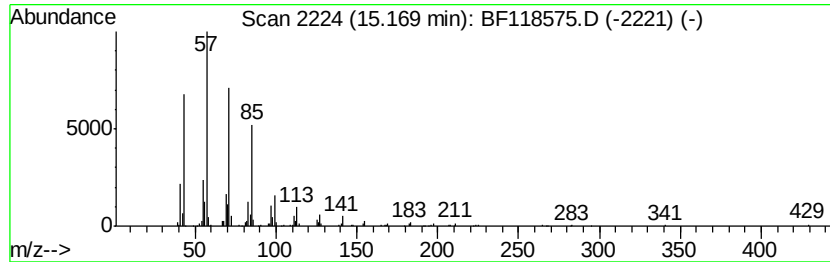
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	2.82 ng	428221	Perylene-d12	15.52

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Hexacosane		366	C26H54	000630-01-3	91
3	Tetracosane		338	C24H50	000646-31-1	91
4	2-methyloctacosane		408	C29H60	1000376-72-8	91
5	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011720\
Data File : BF118575.D
Acq On : 17 Jan 2020 23:14
Operator : JU
Sample : PB126175BL
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB126175BL

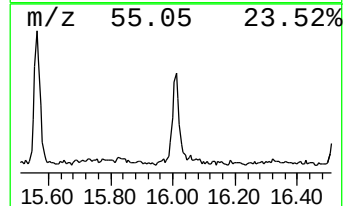
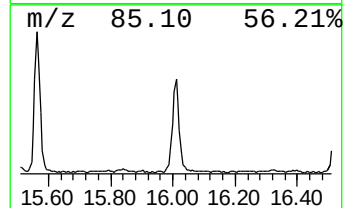
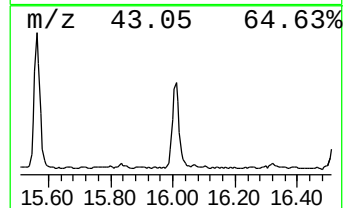
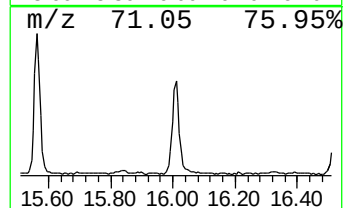
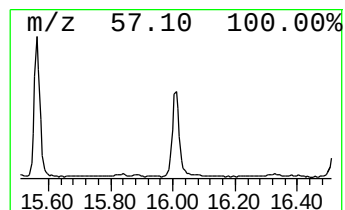
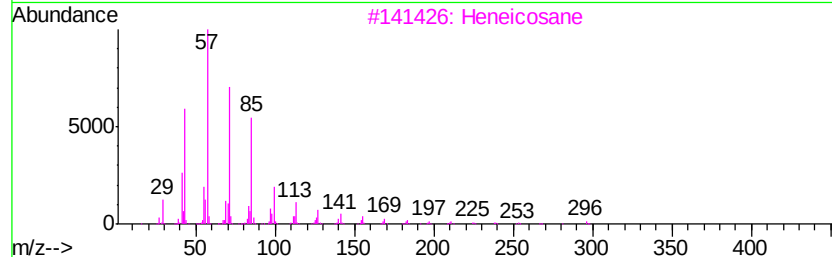
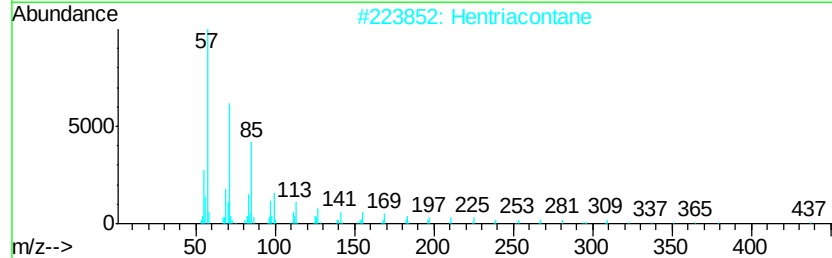
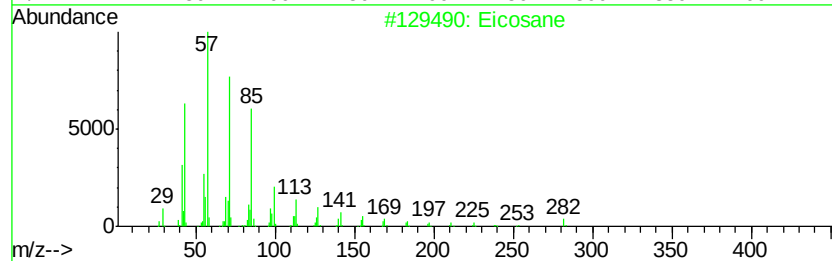
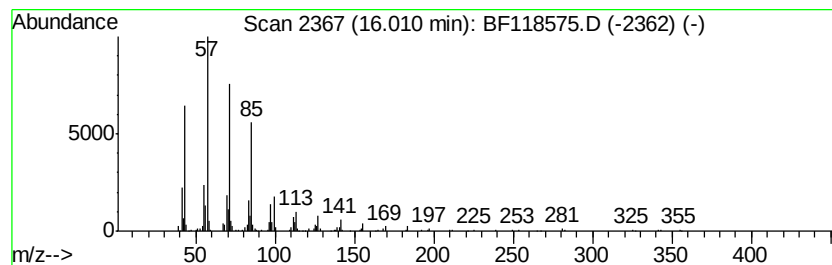
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.01	2.40 ng	365421	Perylene-d12	15.52

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	95
2	Hentriacontane		437	C31H64	000630-04-6	91
3	Heneicosane		296	C21H44	000629-94-7	91
4	Tetratetracontane		619	C44H90	007098-22-8	91
5	Hexacosane		366	C26H54	000630-01-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF011720\
Data File : BF118575.D
Acq On : 17 Jan 2020 23:14
Operator : JU
Sample : PB126175BL
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB126175BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011720.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
Butane, 2-methoxy...	2.17	90.5	ng	9366760	1	6.89	2070260	20.0
2-Pentanone, 4-hy...	5.09	2.2	ng	230940	1	6.89	2070260	20.0
unknown6.65	6.65	66.3	ng	6860390	1	6.89	2070260	20.0
Cyclohexasiloxane...	8.70	3.1	ng	401965	2	8.17	2576350	20.0
Cycloheptasiloxan...	9.63	2.5	ng	379978	3	9.92	3096710	20.0
Hexacosane	14.83	2.6	ng	389870	6	15.52	3039530	20.0
Heneicosane	15.17	2.8	ng	428221	6	15.52	3039530	20.0
Eicosane	16.01	2.4	ng	365421	6	15.52	3039530	20.0