

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
 Data File : BF136354.D
 Acq On : 02 Dec 2023 01:12
 Operator : CG\JU
 Sample : 05561-01
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A821

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-BF112723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136354.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	10	rVB	1929669	1901102	40.00%	8.155%
2	5.440	566	570	573	rBV	2021097	1772431	37.29%	7.603%
3	6.434	735	739	742	rBV	1333515	1082016	22.77%	4.642%
4	6.804	798	802	805	rBV	941764	722631	15.20%	3.100%
5	7.369	890	898	901	rBV	2452799	2477711	52.13%	10.629%
6	7.522	920	924	927	rVB	73894	60984	1.28%	0.262%
7	8.081	1014	1019	1022	rBV	1224613	996764	20.97%	4.276%
8	9.163	1197	1203	1206	rBV	5542233	4752723	100.00%	20.388%
9	9.281	1218	1223	1234	rVB	770231	830985	17.48%	3.565%
10	9.839	1314	1318	1321	rBV	1294966	1020677	21.48%	4.379%
11	10.633	1448	1453	1456	rBV	2302319	2187770	46.03%	9.385%
12	11.327	1567	1571	1575	rBV	1014814	805750	16.95%	3.457%
13	11.869	1659	1663	1668	rBV2	111765	131488	2.77%	0.564%
14	12.445	1758	1761	1767	rVB	64758	64102	1.35%	0.275%
15	12.657	1794	1797	1805	rBV2	48706	54821	1.15%	0.235%
16	12.927	1839	1843	1846	rBV	3280769	2791037	58.73%	11.973%
17	13.980	2018	2022	2029	rVB	610556	592111	12.46%	2.540%
18	14.468	2101	2105	2111	rBV3	48747	58934	1.24%	0.253%
19	14.863	2167	2172	2177	rBV4	54138	78274	1.65%	0.336%
20	15.304	2243	2247	2255	rVB3	47355	68928	1.45%	0.296%
21	15.462	2269	2274	2281	rBV	486219	644135	13.55%	2.763%
22	15.827	2329	2336	2341	rBV4	38297	73610	1.55%	0.316%
23	16.451	2434	2442	2448	rBV4	29269	69216	1.46%	0.297%
24	17.198	2563	2569	2579	rVB5	27342	72864	1.53%	0.313%

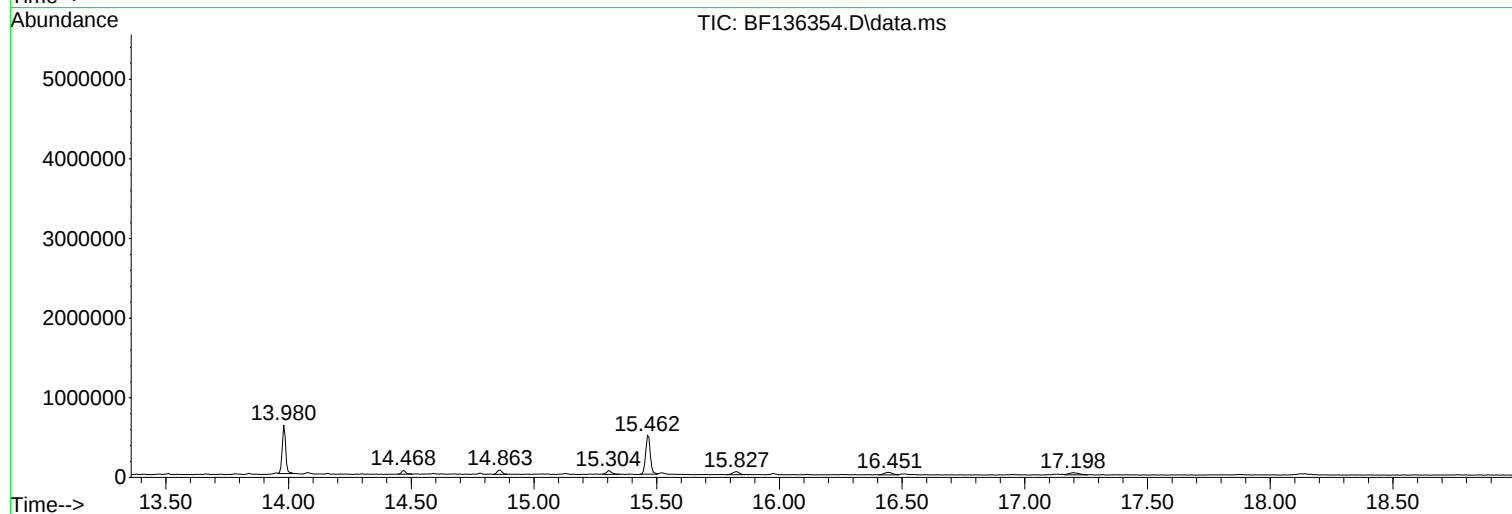
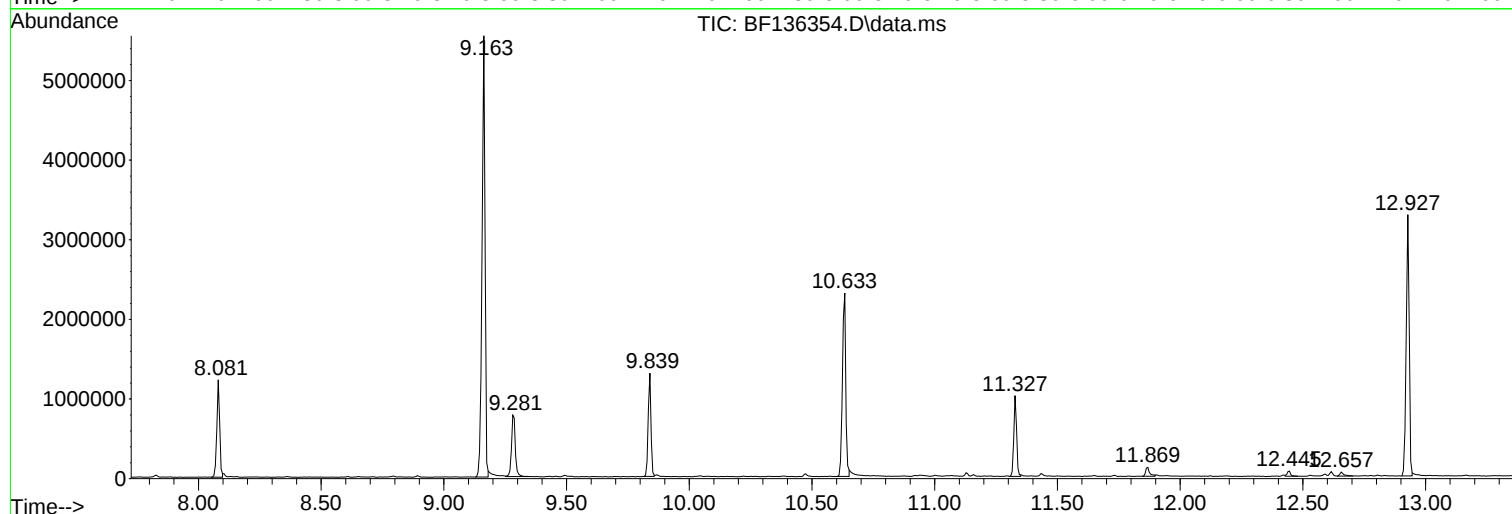
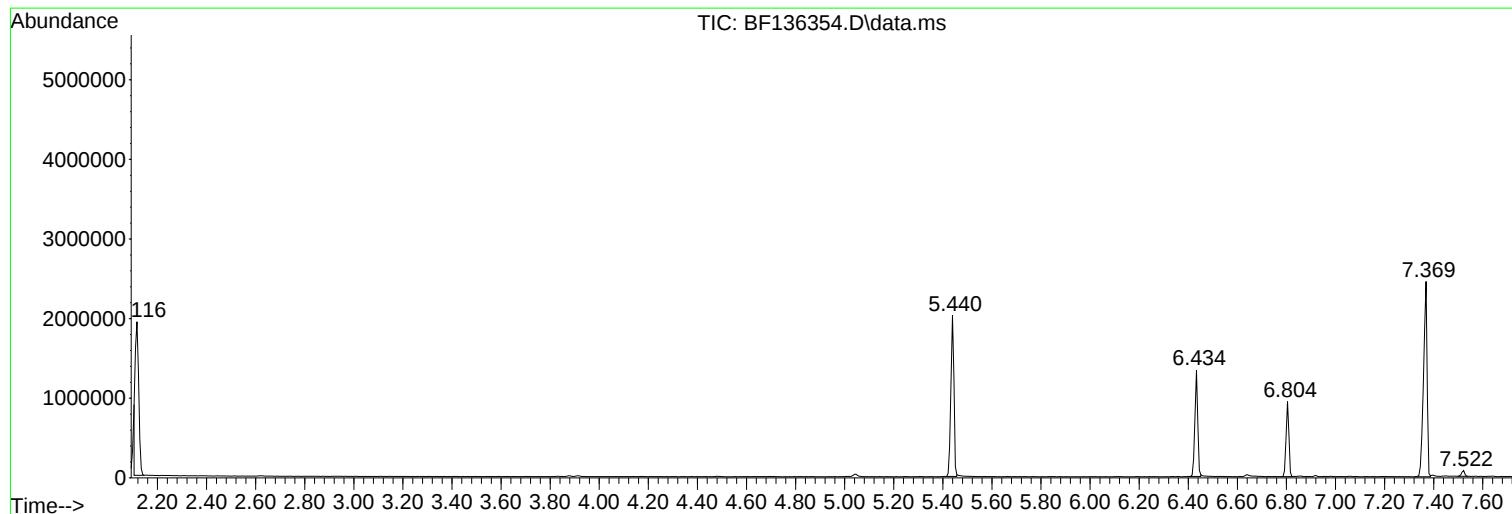
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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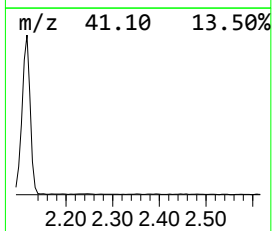
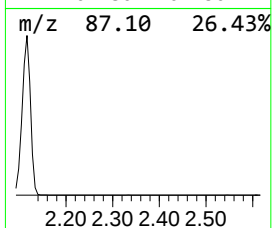
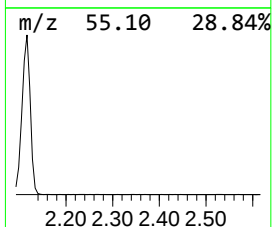
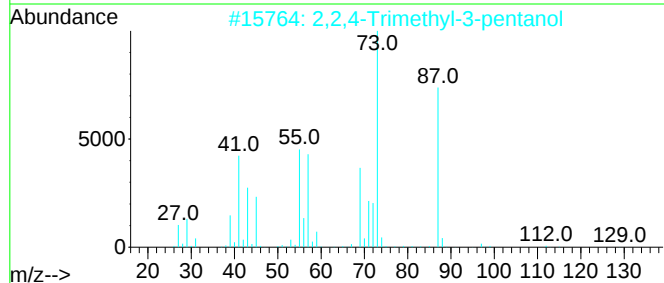
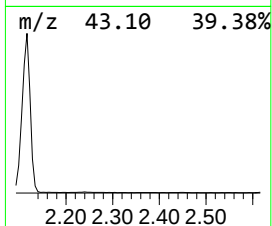
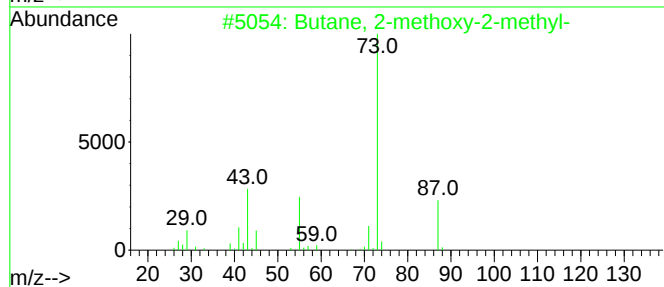
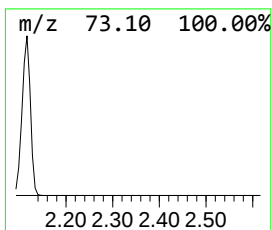
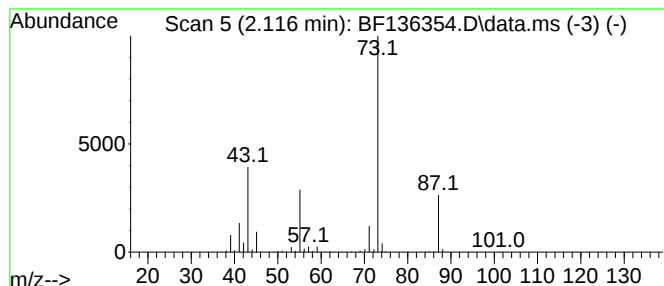
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	52.62 ng	1901100	1,4-Dichlorobenzene-d4	6.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	16
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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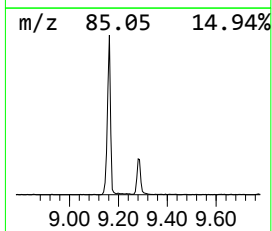
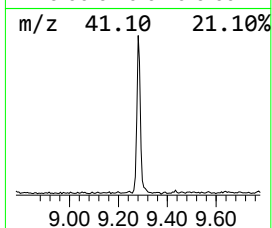
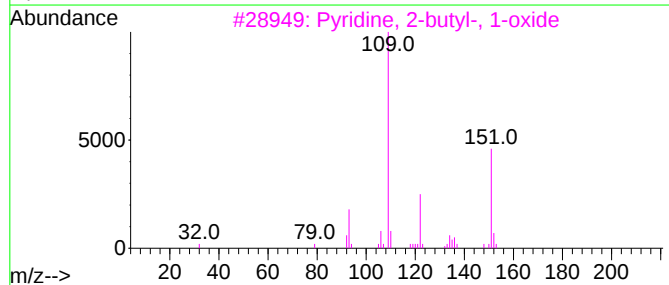
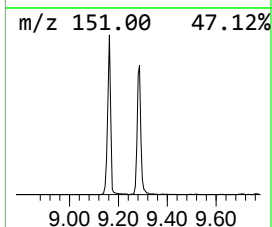
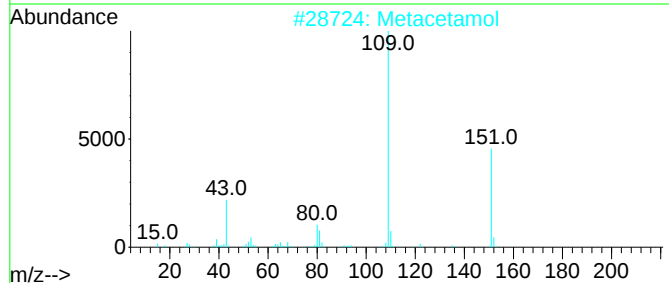
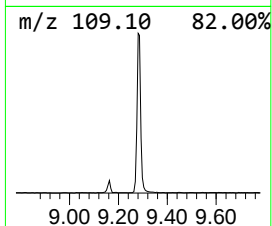
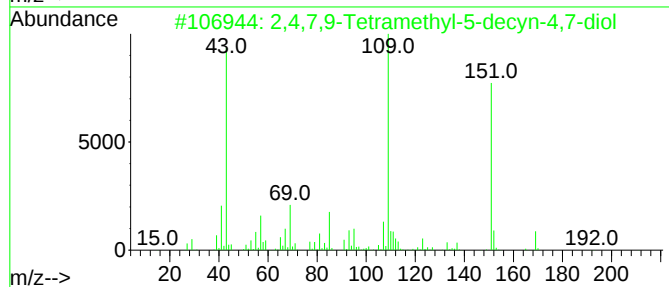
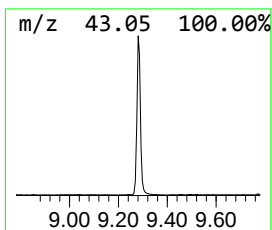
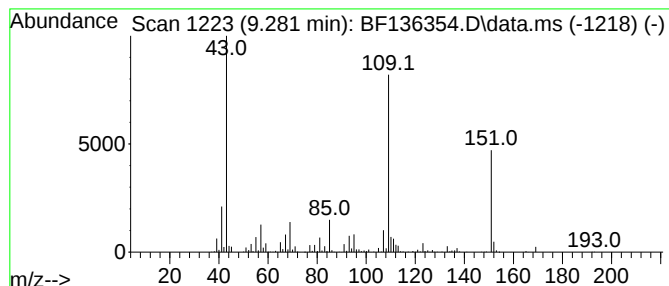
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Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.
9.281	16.28 ng	830985	Acenaphthene-d10		9.839

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	62	
2	Metacetamol	151	C8H9NO2	000621-42-1	59	
3	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59	
4	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	45	
5	Acetaminophen	151	C8H9NO2	000103-90-2	45	



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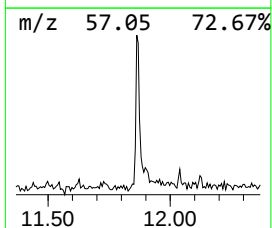
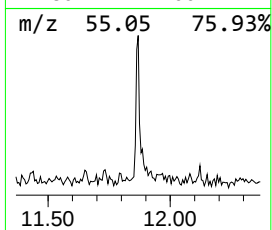
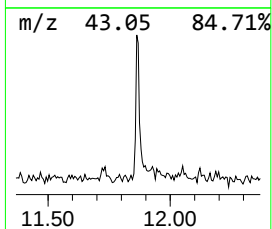
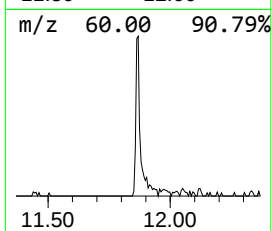
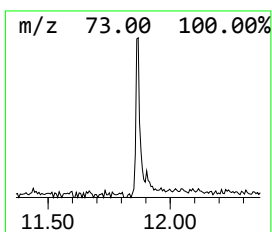
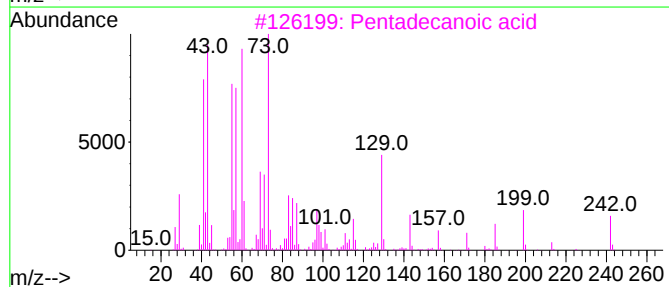
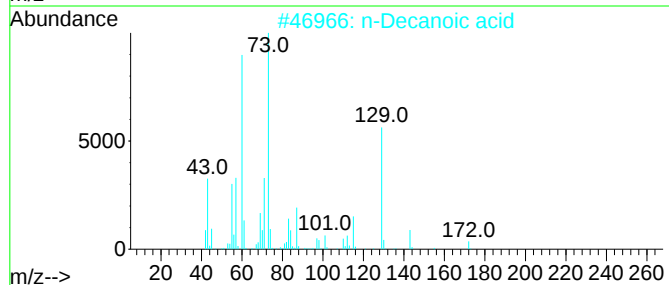
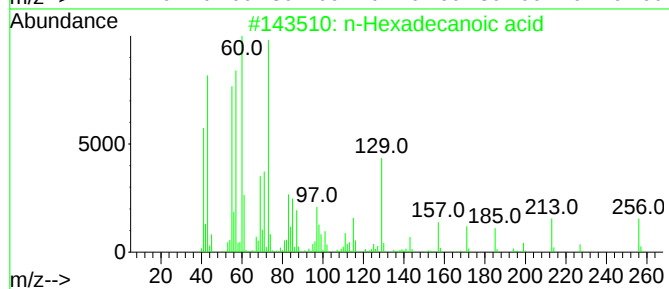
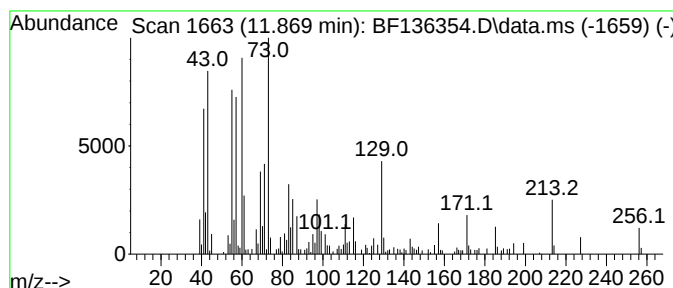
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.869	3.26 ng	131488	Phenanthrene-d10	11.327	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	n-Decanoic acid	172	C10H20O2	000334-48-5	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	Undecanoic acid	186	C11H22O2	000112-37-8	58



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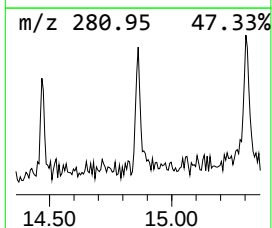
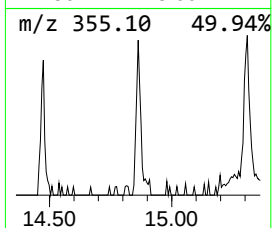
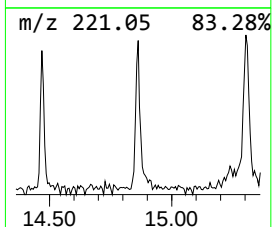
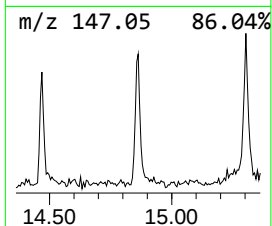
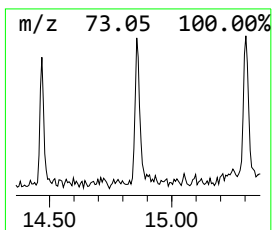
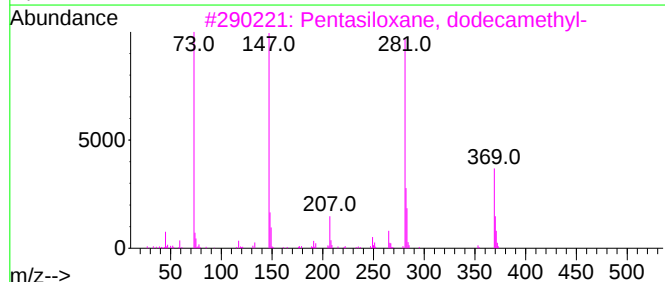
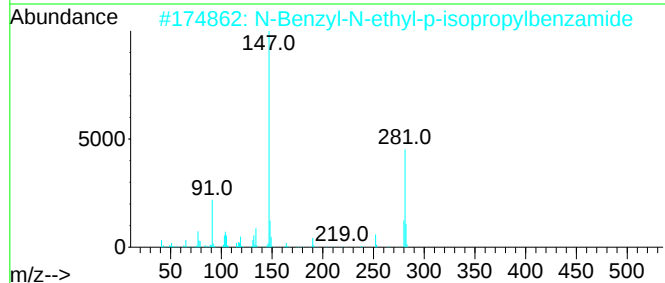
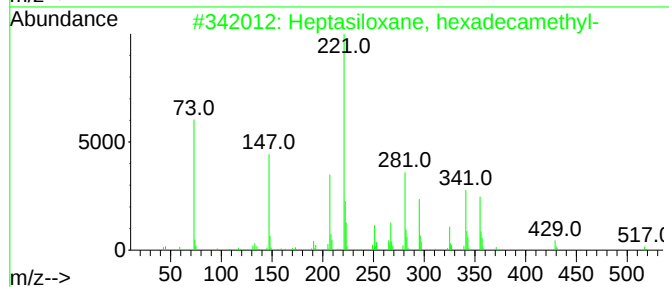
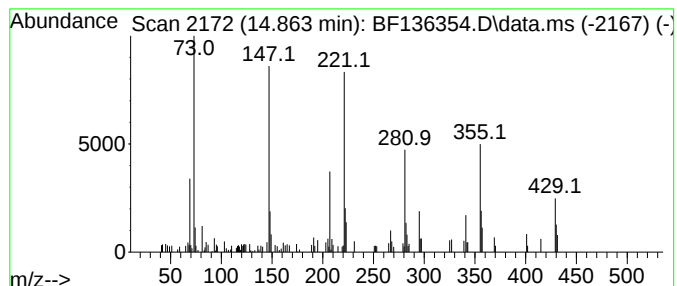
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Peak Number 4 Heptasiloxane, hexadecamethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.863	2.43 ng	78274	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	72
2			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	25
3			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	25
4			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	22
5			benzenamine, N-[bis(2,4,6-trimet...	341	C24H28BN	1000398-20-2	18



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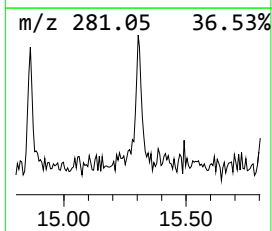
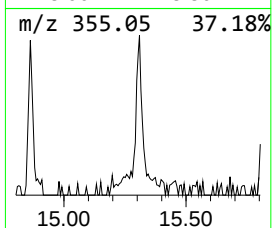
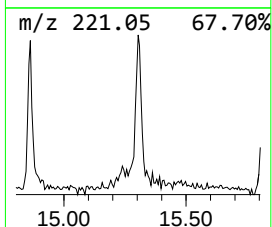
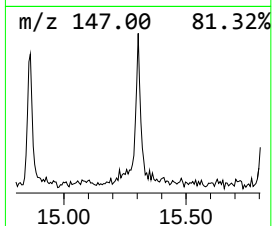
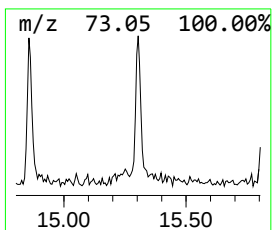
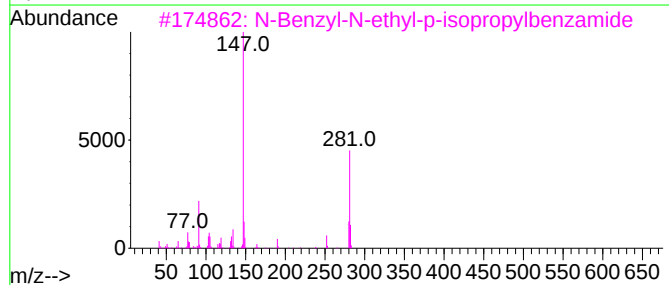
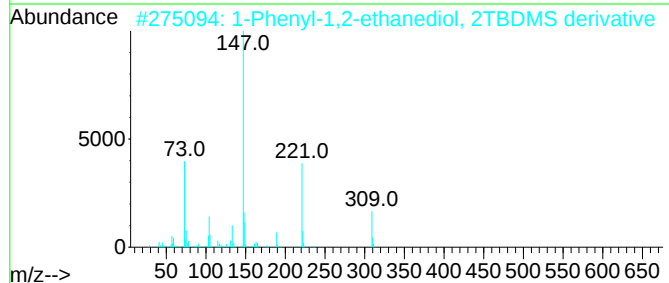
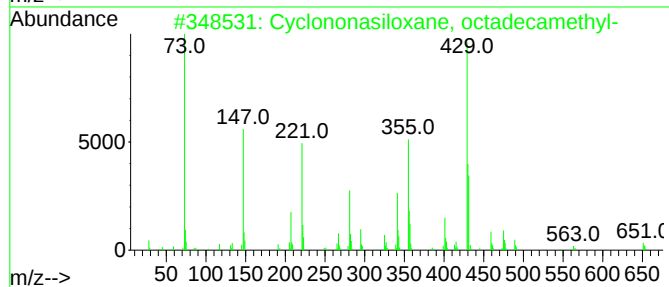
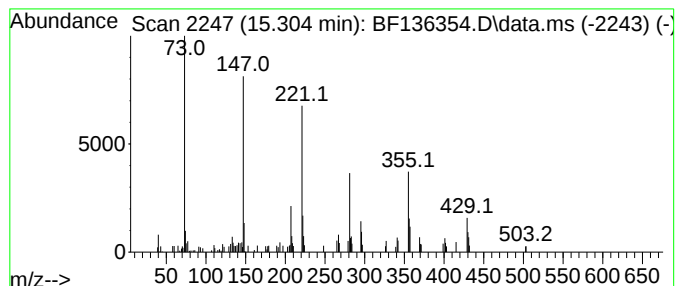
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Peak Number 5 Cyclononasiloxane, octadeca... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.304	2.14 ng	68928	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	91
2			1-Phenyl-1,2-ethanediol, 2TBDMS ...	366	C20H38O2Si2	1000373-40-4	47
3			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	38
4			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	38
5			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	38



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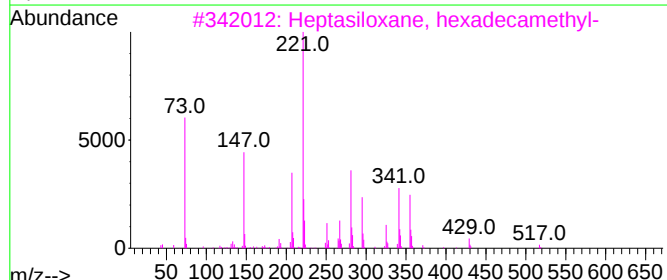
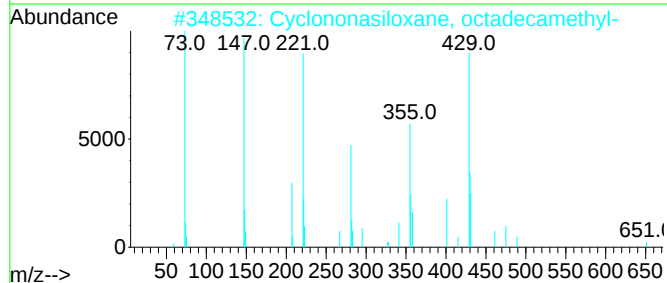
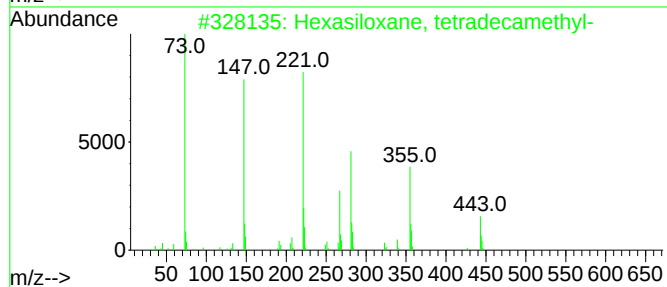
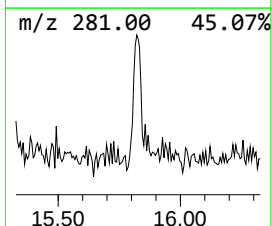
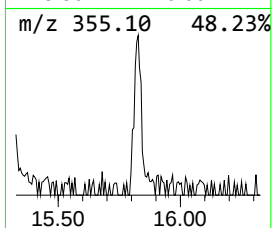
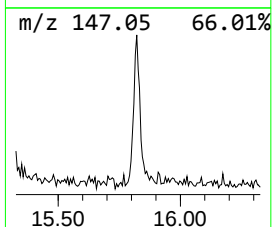
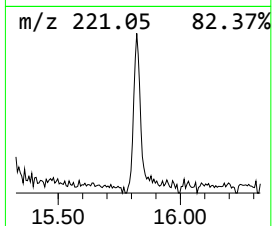
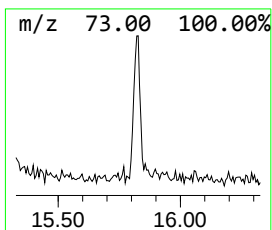
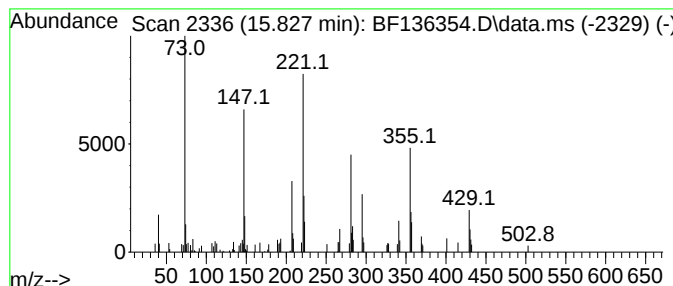
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexasiloxane, tetradecamethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.827	2.29 ng	73610	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	52
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	50
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	50
4			3,6-Dioxo-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	38
5			7-Methylimidazo[1,2-a]pyrimidin...	221	C10H15N3OSi	1010468-48-3	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
Data File : BF136354.D
Acq On : 02 Dec 2023 01:12
Operator : CG\JU
Sample : 05561-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A821

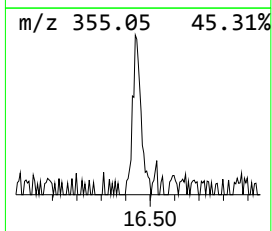
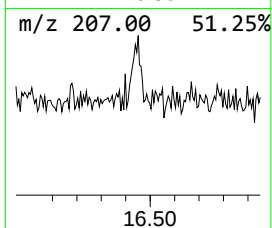
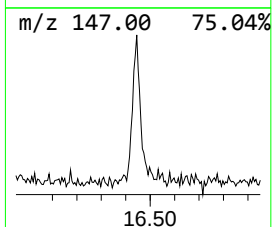
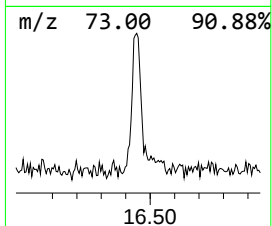
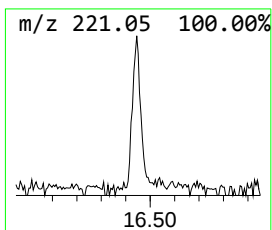
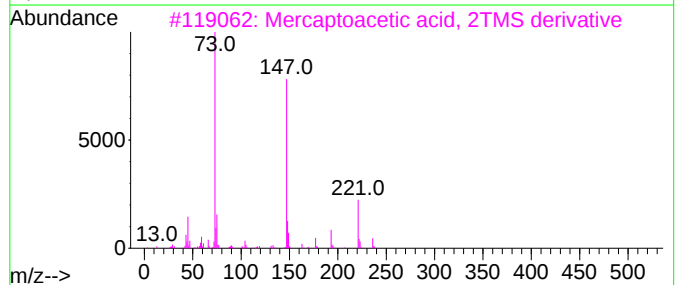
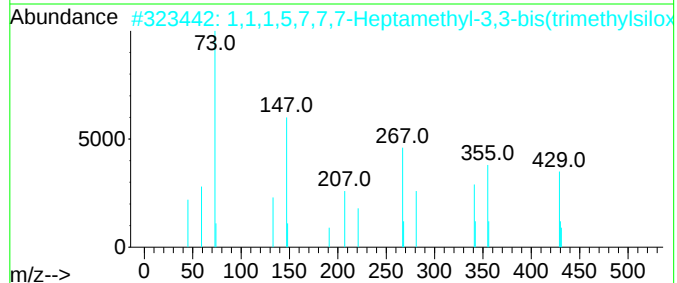
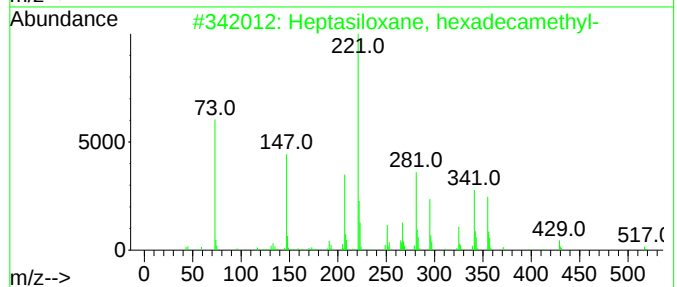
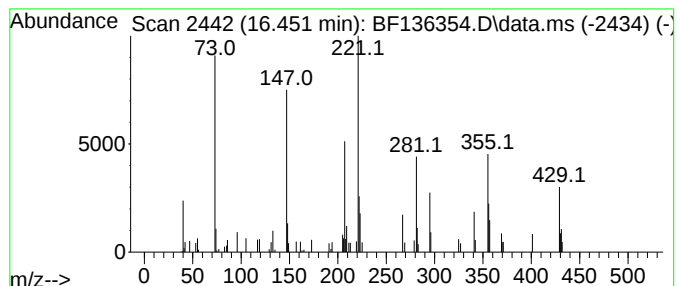
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown16.451 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.451	2.15 ng	69216	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	42
2			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	38
3			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	25
4			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	18
5			Trisiloxane, octamethyl-	236	C8H24O2Si3	000107-51-7	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
Data File : BF136354.D
Acq On : 02 Dec 2023 01:12
Operator : CG\JU
Sample : 05561-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A821

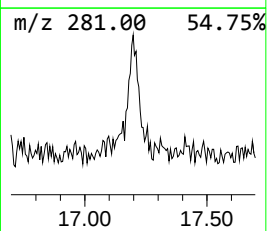
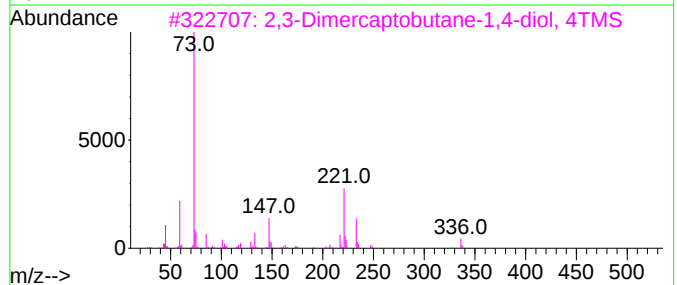
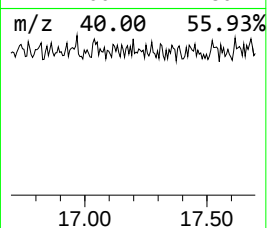
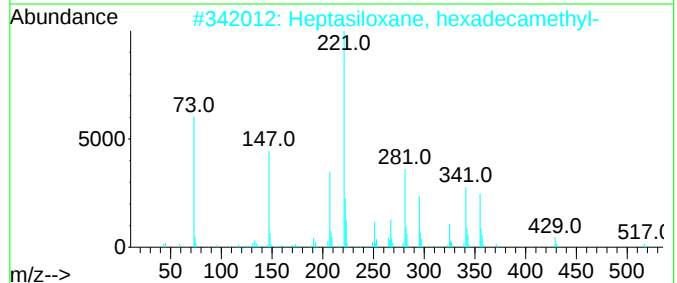
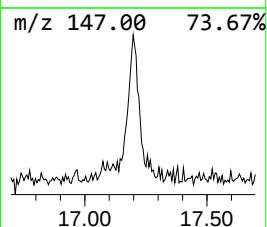
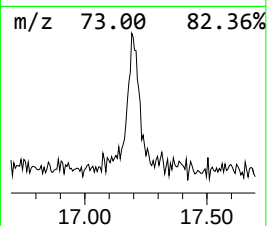
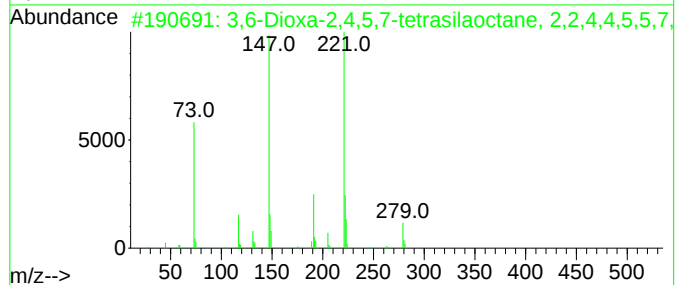
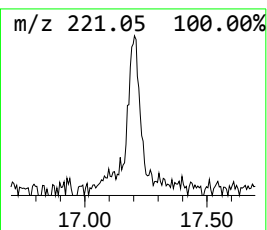
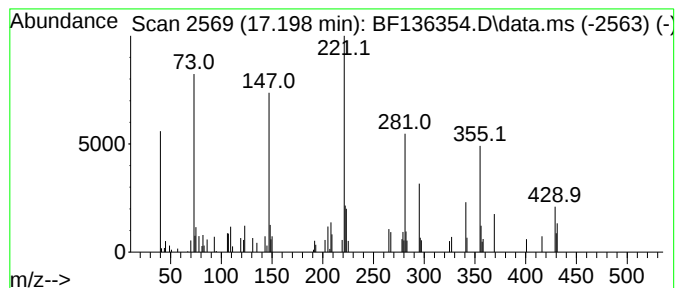
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown17.198 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.198	2.26 ng	72864	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	46
2			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	46
3			2,3-Dimercaptobutane-1,4-diol, 4TMS	442	C16H42O2S2Si4	959295-06-8	32
4			2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	32
5			Trimethylsilyl 4-propylbenzoate	236	C13H20O2Si	1000408-13-2	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
Data File : BF136354.D
Acq On : 02 Dec 2023 01:12
Operator : CG\JU
Sample : 05561-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A821

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.116	52.6	ng	1901100	1	6.804	722631	20.0
2,4,7,9-Tetrame...	9.281	16.3	ng	830985	3	9.839	1020680	20.0
n-Hexadecanoic ...	11.869	3.3	ng	131488	4	11.327	805750	20.0
Heptasiloxane, ...	14.863	2.4	ng	78274	6	15.463	644135	20.0
Cyclononasiloxa...	15.304	2.1	ng	68928	6	15.463	644135	20.0
Hexasiloxane, t...	15.827	2.3	ng	73610	6	15.463	644135	20.0
unknown16.451	16.451	2.1	ng	69216	6	15.463	644135	20.0
unknown17.198	17.198	2.3	ng	72864	6	15.463	644135	20.0