

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
 Data File : BF136743.D
 Acq On : 27 Dec 2023 03:46
 Operator : CG\JU
 Sample : 05602-03
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SPRING-VALLEY-TP-2

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136743.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	11	15	22	rVB	16570	22875	1.69%	0.234%
2	5.022	495	499	507	rVB	54961	70065	5.19%	0.718%
3	5.428	564	568	571	rBV	1600495	1350396	100.00%	13.843%
4	6.428	734	738	741	rBV	1341181	1316697	97.50%	13.497%
5	6.781	795	798	802	rBV	475137	395055	29.25%	4.050%
6	7.345	889	894	897	rBV	972445	833074	61.69%	8.540%
7	7.951	994	997	1002	rVB	68708	51683	3.83%	0.530%
8	8.057	1012	1015	1019	rBV	505455	451175	33.41%	4.625%
9	9.139	1194	1199	1202	rBV	1486960	1319617	97.72%	13.527%
10	9.816	1310	1314	1318	rBV	528325	406429	30.10%	4.166%
11	10.610	1445	1449	1452	rBV	775557	658569	48.77%	6.751%
12	11.310	1564	1568	1571	rBV	444348	409708	30.34%	4.200%
13	11.845	1655	1659	1669	rBV2	123641	151471	11.22%	1.553%
14	12.527	1771	1775	1778	rBV	52326	48026	3.56%	0.492%
15	12.557	1778	1780	1788	rVB9	10518	19210	1.42%	0.197%
16	12.633	1790	1793	1797	rBV3	36997	39186	2.90%	0.402%
17	12.757	1809	1814	1816	rBV	46084	42164	3.12%	0.432%
18	12.904	1835	1839	1842	rBV	1437904	1220569	90.39%	12.512%
19	13.080	1863	1869	1873	rBV8	15610	31837	2.36%	0.326%
20	13.339	1911	1913	1917	rBV5	12024	17582	1.30%	0.180%
21	13.810	1991	1993	1997	rBV4	17514	23469	1.74%	0.241%
22	13.963	2015	2019	2022	rBV	441473	405778	30.05%	4.160%
23	14.433	2096	2099	2103	rVB3	43845	53333	3.95%	0.547%
24	14.815	2162	2164	2169	rVB2	59373	66284	4.91%	0.679%
25	15.251	2235	2238	2243	rVB2	58960	83338	6.17%	0.854%
26	15.445	2267	2271	2279	rVB	204957	267698	19.82%	2.744%

Sum of corrected areas: 9755288

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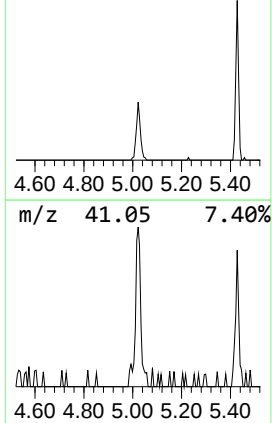
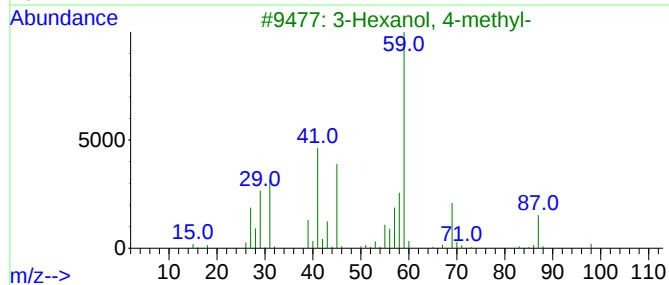
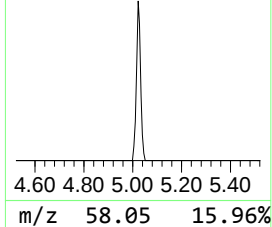
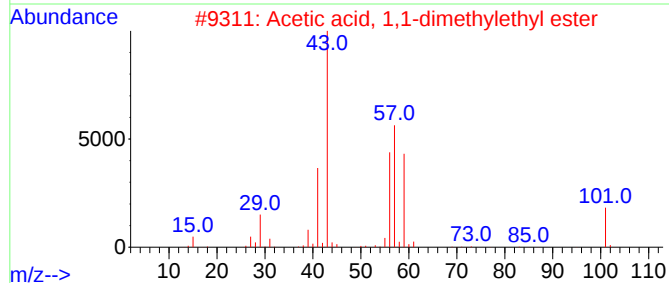
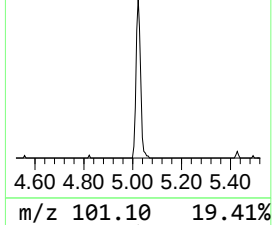
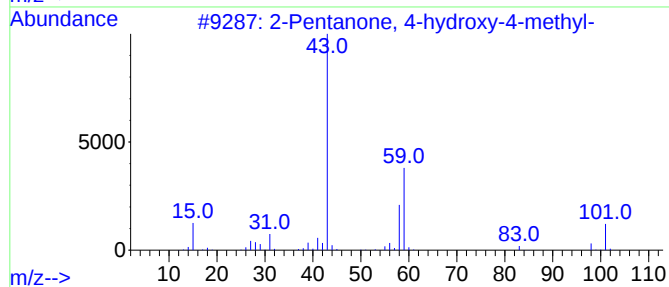
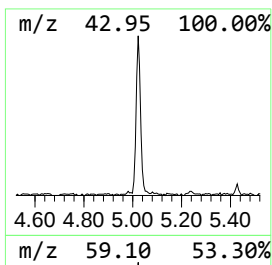
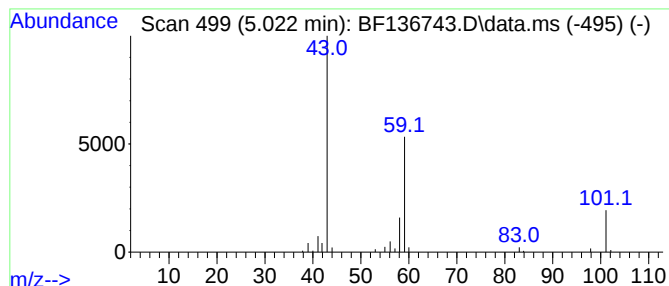
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	3.55 ng	70065	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9		



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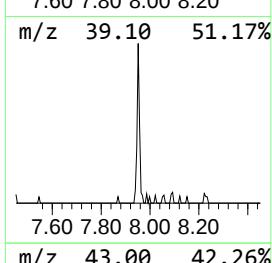
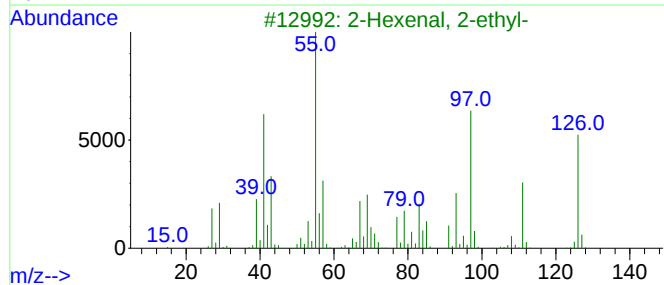
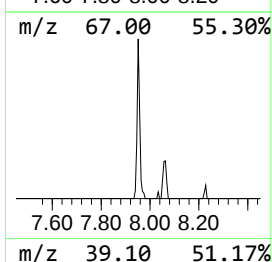
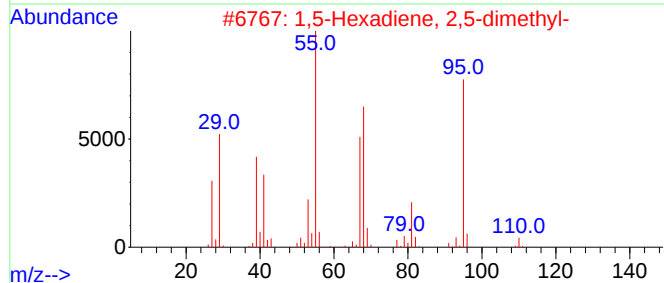
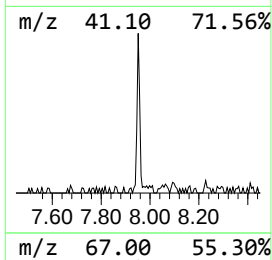
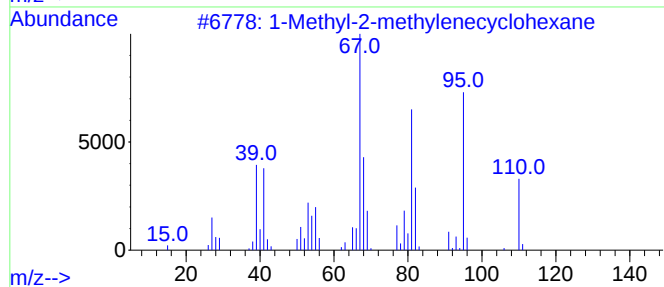
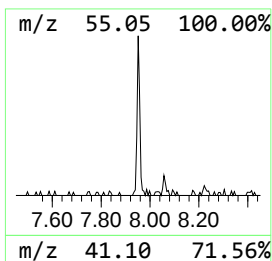
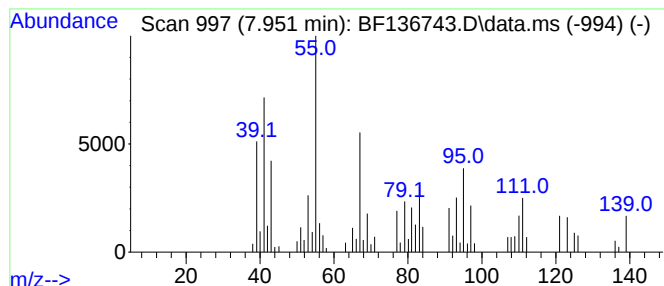
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown7.951 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.951	2.29 ng	51683	Naphthalene-d8	8.063

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Methyl-2-methylenecyclohexane	110	C8H14	002808-75-5	38
2		1,5-Hexadiene, 2,5-dimethyl-	110	C8H14	000627-58-7	27
3		2-Hexenal, 2-ethyl-	126	C8H14O	000645-62-5	27
4		9-Oxabicyclo[6.1.0]nonane	126	C8H14O	000286-62-4	25
5		1,4-Octadiene	110	C8H14	005675-25-2	18



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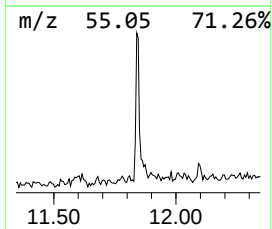
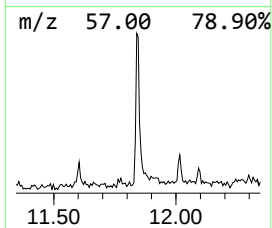
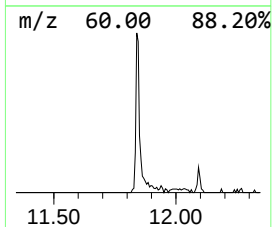
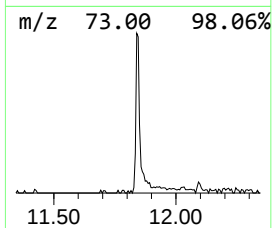
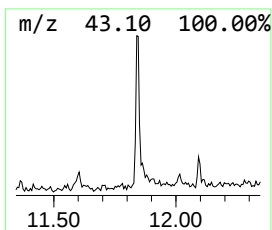
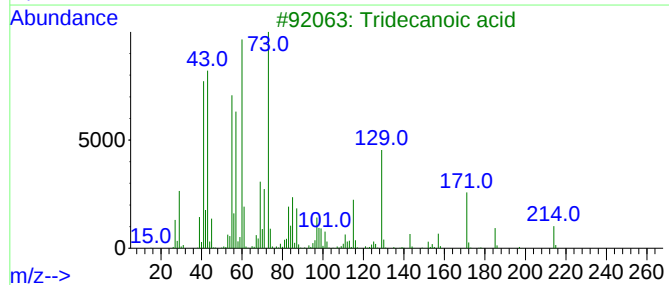
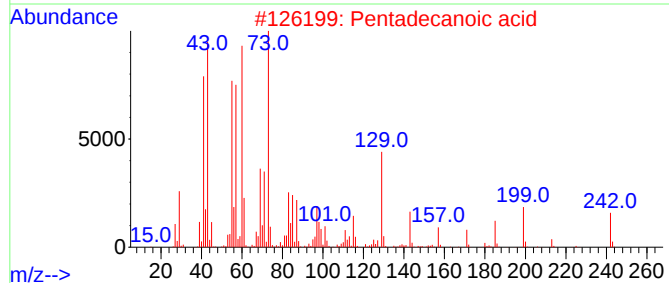
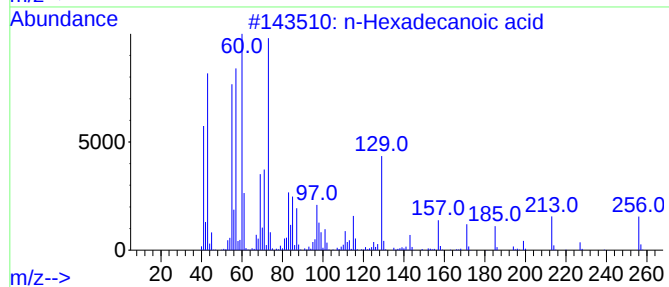
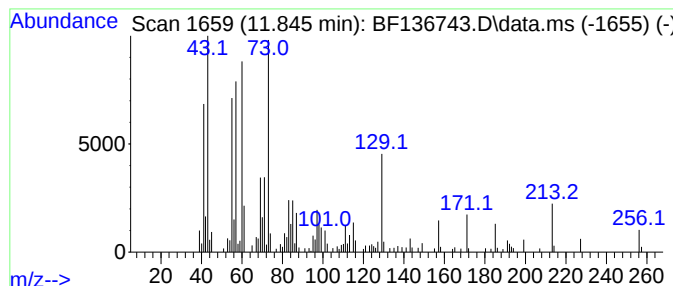
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.845	7.39 ng	151471	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



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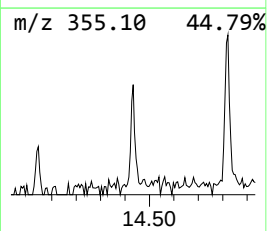
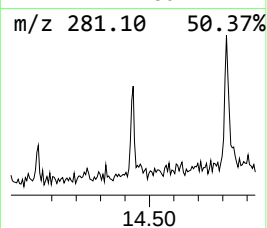
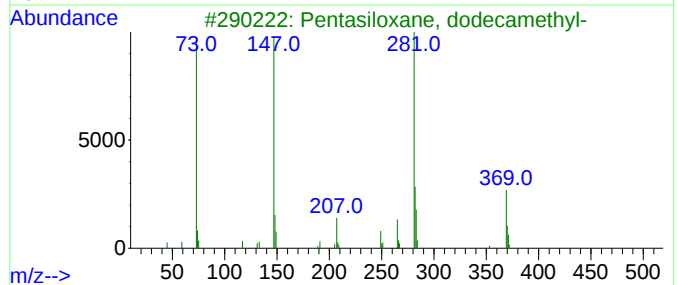
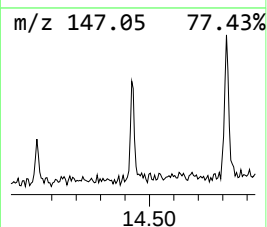
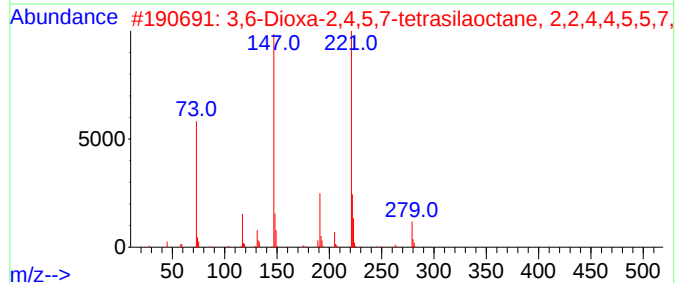
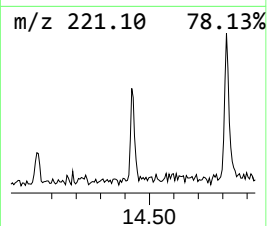
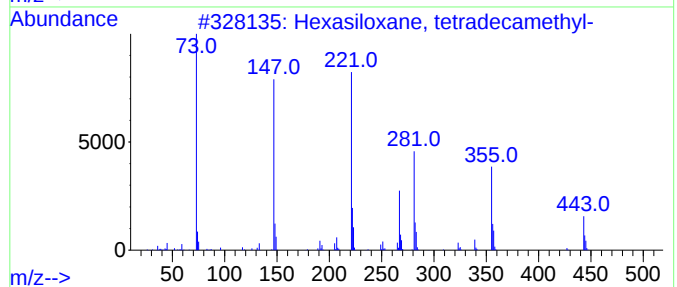
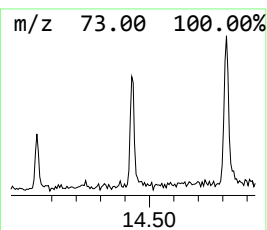
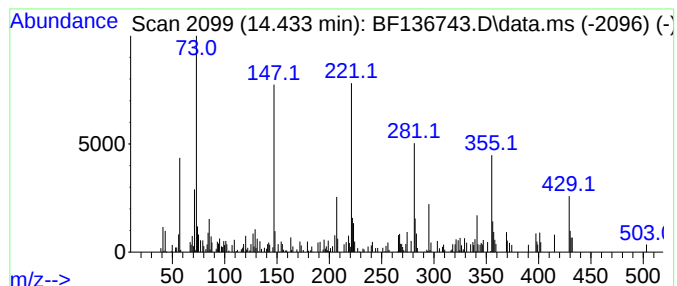
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 Hexasiloxane, tetradecamethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.433	2.63 ng	53333	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	68
2			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	45
3			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	22
4			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	22
5			2-Methyl-6-tert-butylphenol, TMS...	236	C14H24O5Si	1000467-04-9	14



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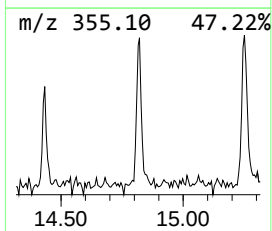
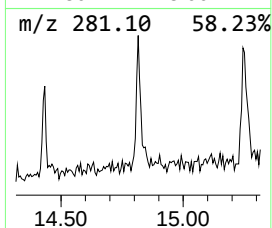
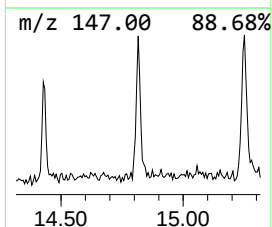
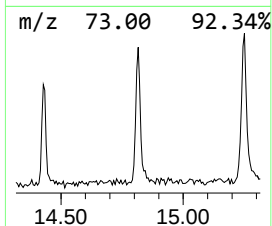
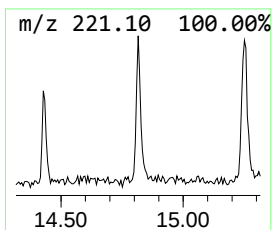
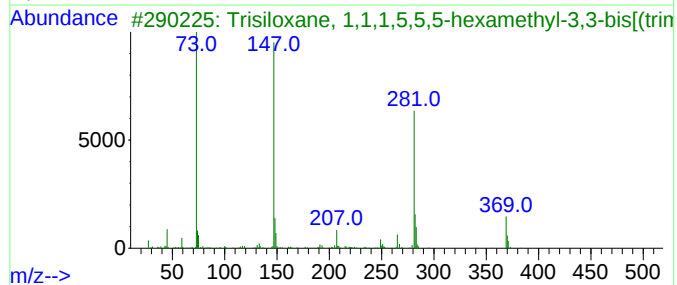
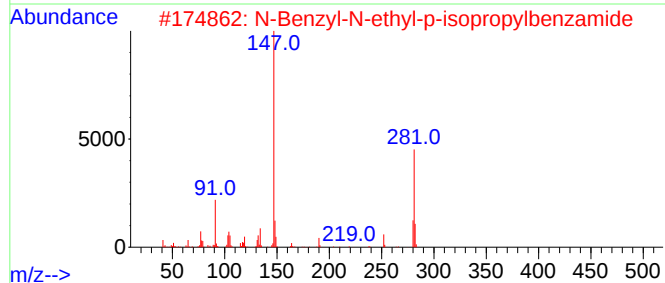
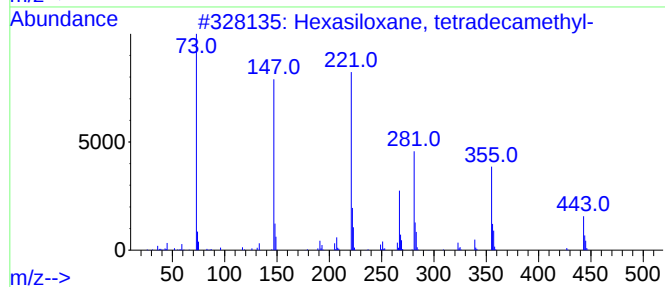
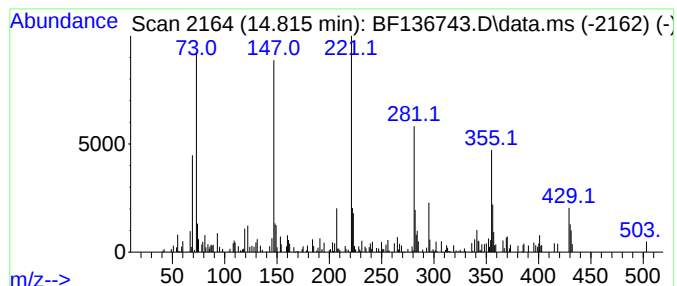
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Peak Number 7 unknown14.816 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.816	4.95 ng	66284	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	68
2			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	22
3			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	22
4			Phthalic acid, 2TMS derivative	310	C14H22O4Si2	002078-22-0	14
5			4,5,6,7-Tetrahydro-2,1-benzisoxa...	282	C13H26N2OSi2	1000478-79-7	11



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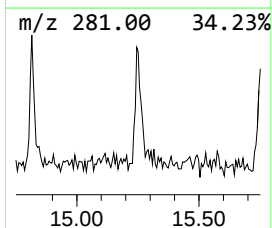
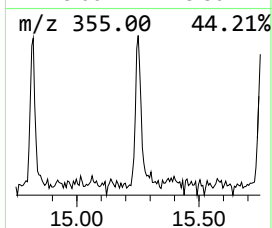
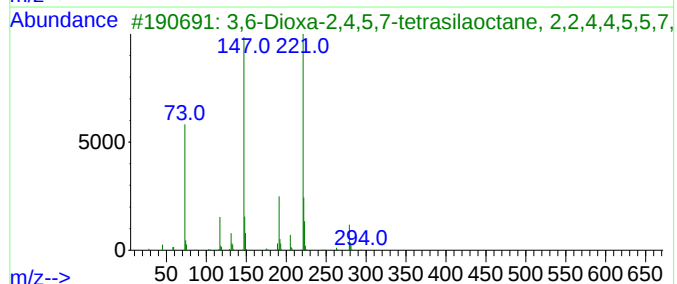
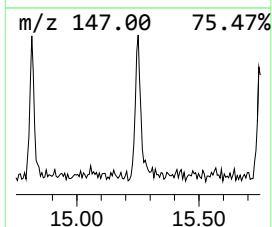
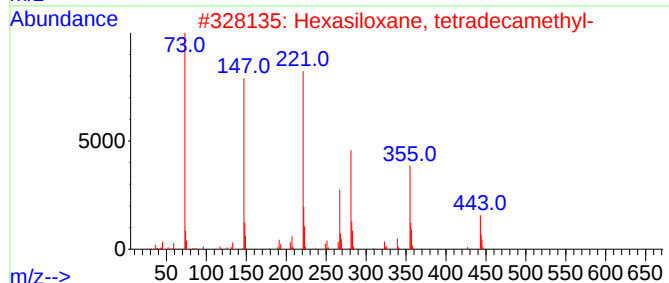
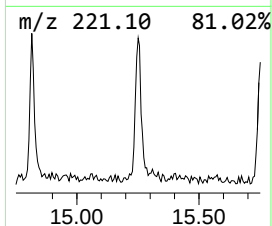
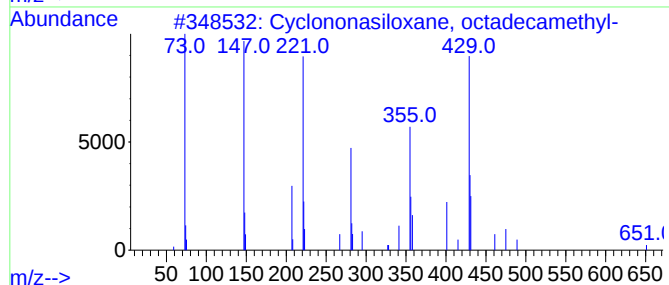
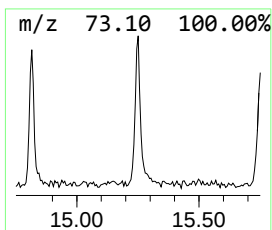
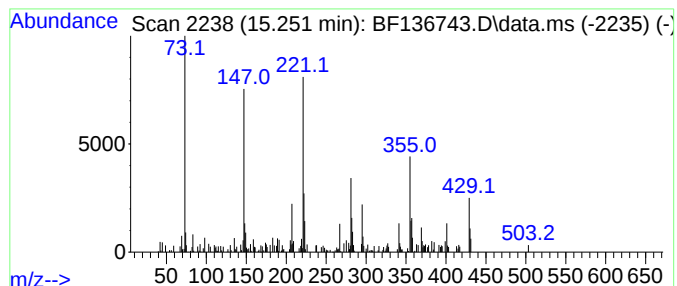
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclononasiloxane, octadeca... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.251	6.23 ng	83338	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	83
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	53
3			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	43
4			4-Hydroxybenzyl alcohol, 2TBDMS ...	352	C19H36O2Si2	1000364-43-9	38
5			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136743.D
Acq On : 27 Dec 2023 03:46
Operator : CG\JU
Sample : 05602-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPRING-VALLEY-TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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
2-Pentanone, 4-...	5.022	3.5	ng	70065	1	6.781	395055	20.0
unknown7.951	7.951	2.3	ng	51683	2	8.063	451175	20.0
n-Hexadecanoic ...	11.845	7.4	ng	151471	4	11.310	409708	20.0
Hexasiloxane, t...	14.433	2.6	ng	53333	5	13.963	405778	20.0
unknown14.816	14.816	5.0	ng	66284	6	15.445	267698	20.0
Cyclononasiloxa...	15.251	6.2	ng	83338	6	15.445	267698	20.0