

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121622\
 Data File : BF131666.D
 Acq On : 16 Dec 2022 14:52
 Operator : CG\JU
 Sample : N6038-17
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RB-37-(3-5)

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-BF120822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131666.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	8	16	rVB	302795	360282	20.82%	2.758%
2	5.087	505	510	518	rVB	219796	267944	15.48%	2.051%
3	5.493	575	579	582	rBV	1560674	1343245	77.63%	10.282%
4	6.510	747	752	755	rBV	1498803	1398474	80.82%	10.704%
5	6.881	811	815	818	rBV	531908	424621	24.54%	3.250%
6	7.445	906	911	914	rBV	1065826	896305	51.80%	6.861%
7	8.169	1030	1034	1037	rBV	657760	527992	30.51%	4.041%
8	9.245	1213	1217	1221	rBV	1797546	1690671	97.70%	12.941%
9	9.934	1330	1334	1337	rBV	687987	608556	35.17%	4.658%
10	10.651	1452	1456	1459	rBV	448431	384447	22.22%	2.943%
11	10.722	1464	1468	1472	rBV	1148480	996880	57.61%	7.630%
12	11.428	1584	1588	1590	rBV	773291	641639	37.08%	4.911%
13	11.451	1590	1592	1595	rVB	34352	26225	1.52%	0.201%
14	12.645	1791	1795	1798	rBV	97390	85291	4.93%	0.653%
15	12.875	1828	1834	1839	rBV	80091	78470	4.53%	0.601%
16	13.022	1854	1859	1862	rBV	1997835	1730412	100.00%	13.245%
17	13.922	2009	2012	2016	rBV3	52458	93484	5.40%	0.716%
18	14.080	2033	2039	2042	rBV	557843	540023	31.21%	4.133%
19	14.104	2042	2043	2049	rVB	56202	33772	1.95%	0.258%
20	14.174	2051	2055	2060	rVB2	27462	32350	1.87%	0.248%
21	14.545	2115	2118	2122	rBV3	28608	29772	1.72%	0.228%
22	14.939	2180	2185	2190	rBV	76851	79487	4.59%	0.608%
23	15.133	2214	2218	2226	rBV	39185	78857	4.56%	0.604%
24	15.210	2227	2231	2235	rVB	48072	52433	3.03%	0.401%
25	15.451	2268	2272	2278	rVB	25938	34082	1.97%	0.261%
26	15.516	2279	2283	2289	rVB	27093	34684	2.00%	0.265%
27	15.580	2289	2294	2303	rBV	320183	416546	24.07%	3.188%
28	15.821	2329	2335	2341	rVB5	25957	40099	2.32%	0.307%
29	16.063	2369	2376	2380	rBV2	27904	47426	2.74%	0.363%
30	16.892	2512	2517	2525	rBV5	19134	36678	2.12%	0.281%
31	17.092	2546	2551	2558	rBV3	14548	29122	1.68%	0.223%
32	17.551	2623	2629	2636	rBV2	12135	24362	1.41%	0.186%

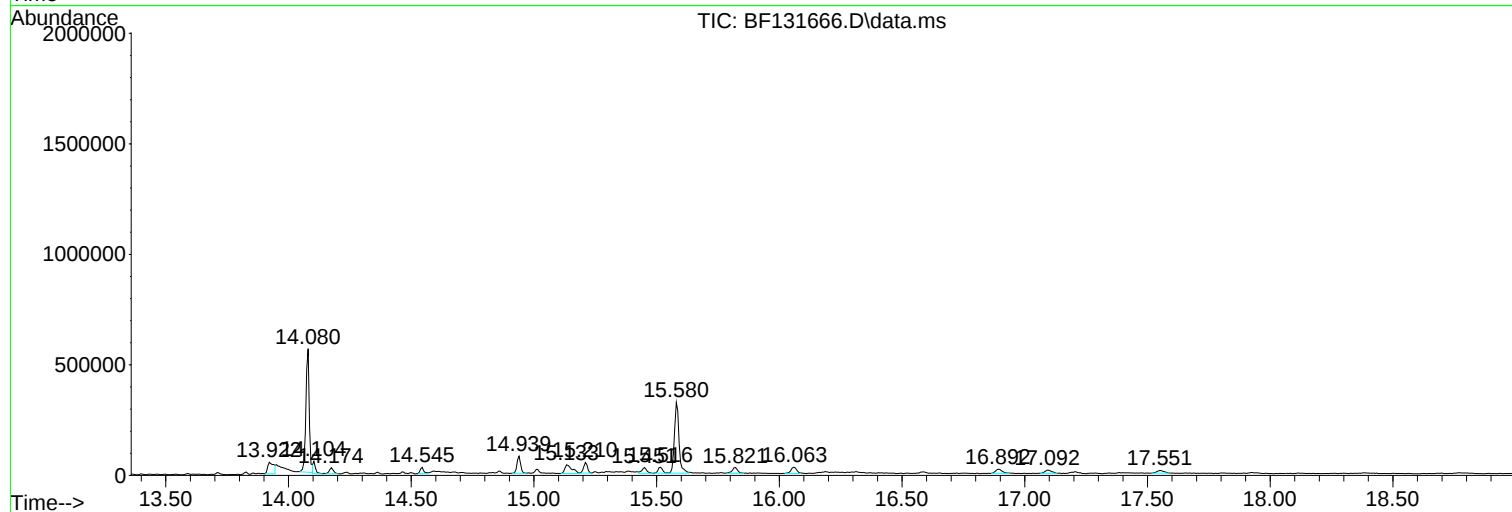
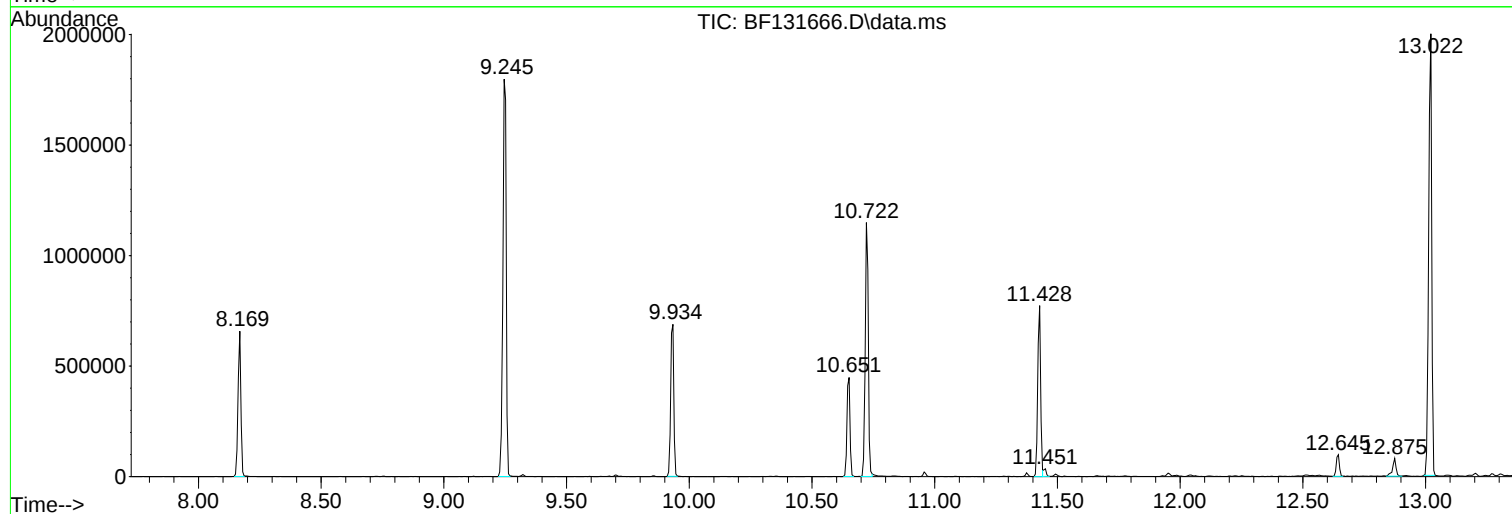
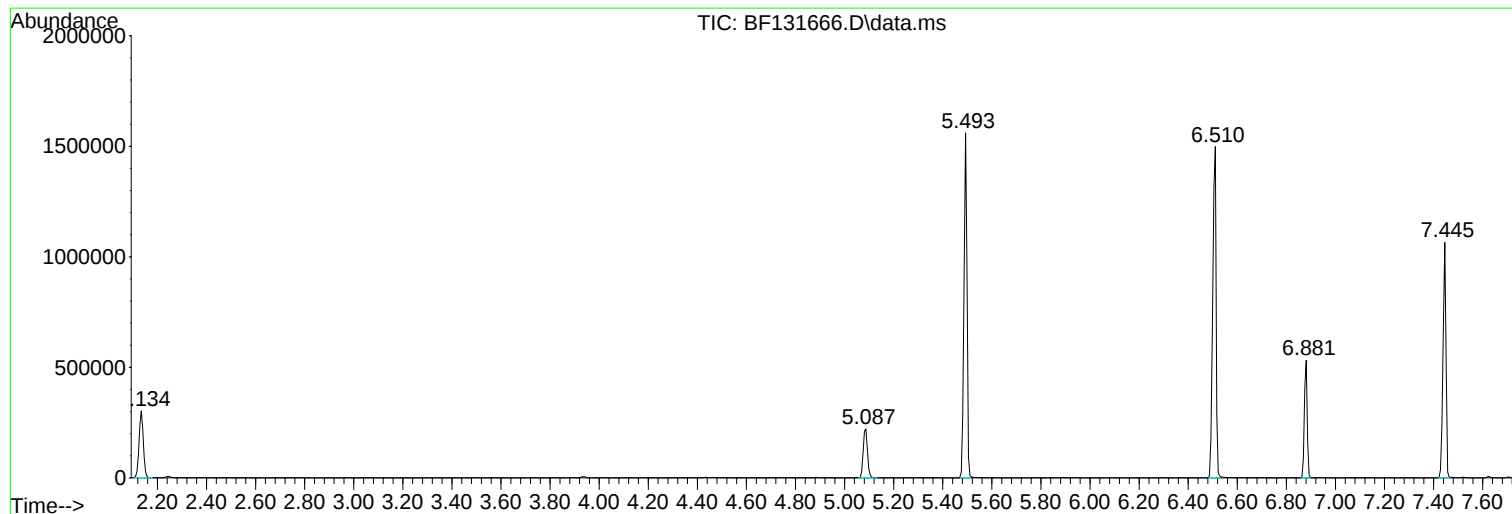
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ClientSampleId :
RB-37-(3-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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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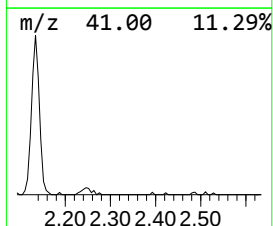
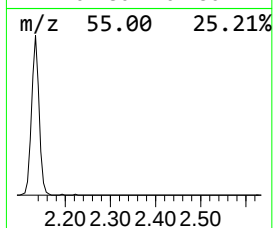
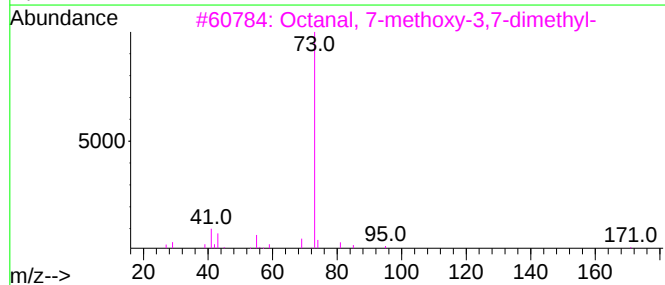
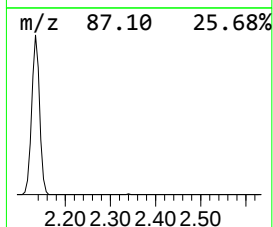
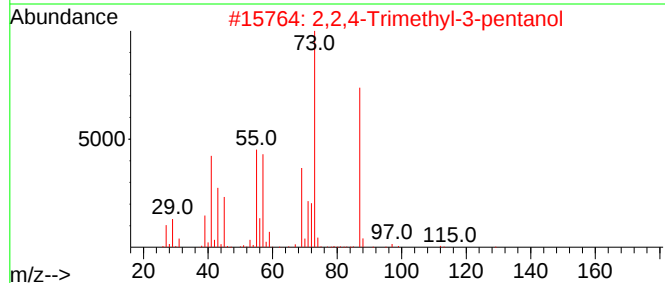
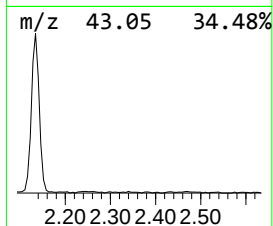
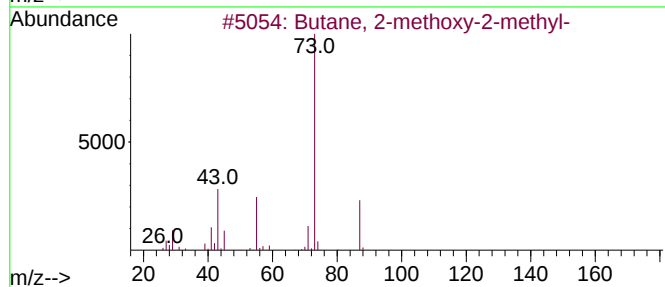
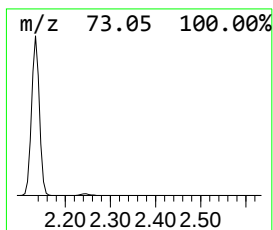
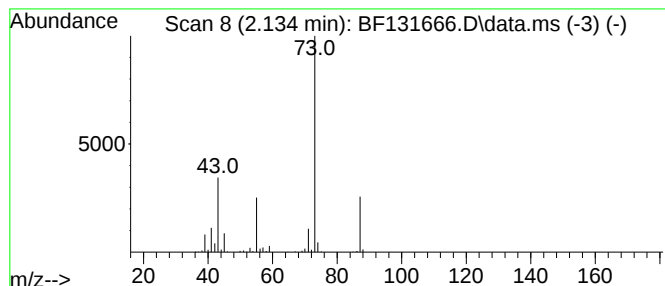
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.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.
2.134	16.97 ng	360282	1,4-Dichlorobenzene-d4	6.881

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	40
3			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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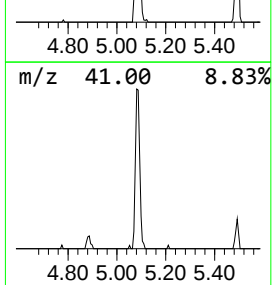
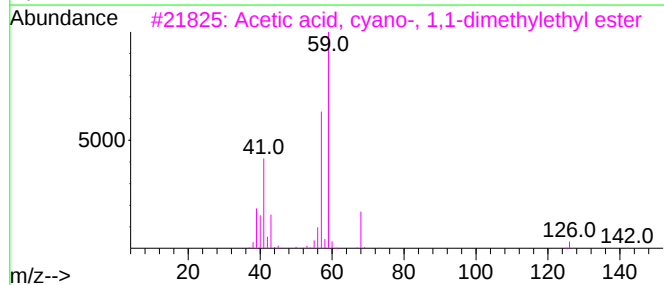
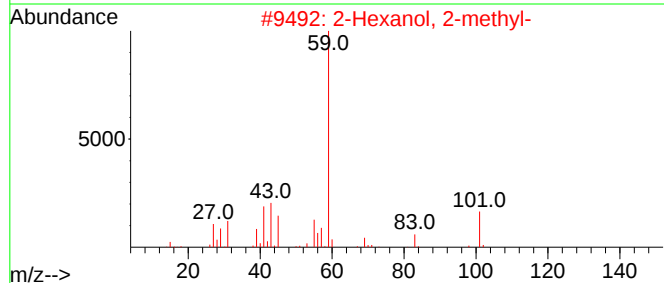
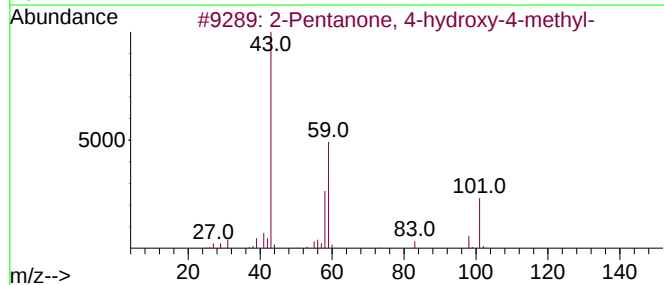
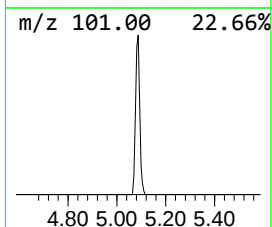
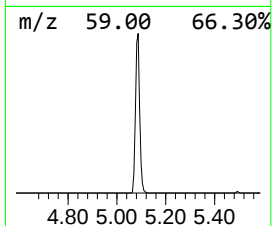
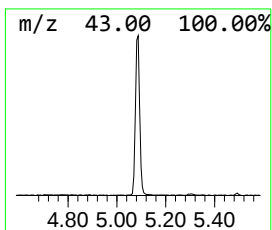
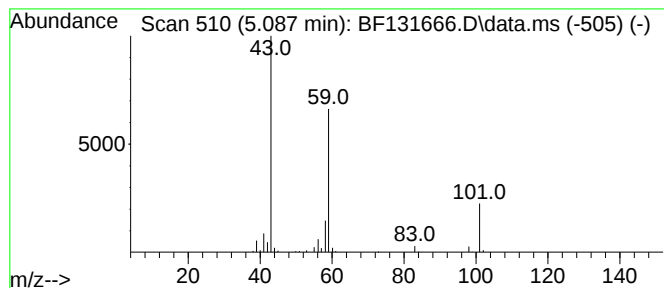
Instrument :
BNA_F
ClientSampleId :
RB-37-(3-5)

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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 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.087	12.62 ng	267944	1,4-Dichlorobenzene-d4	6.881	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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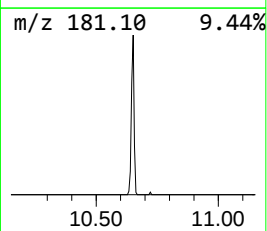
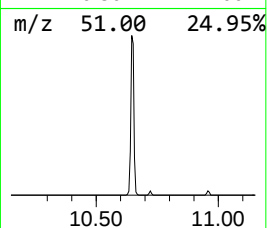
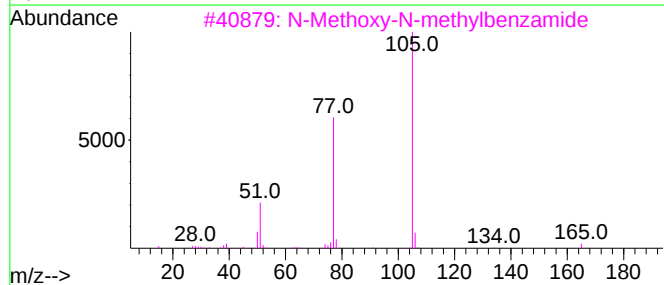
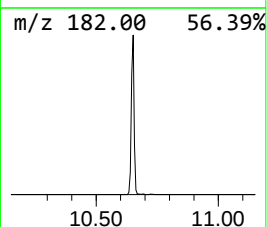
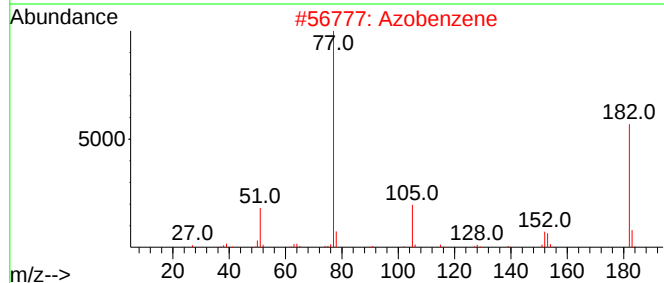
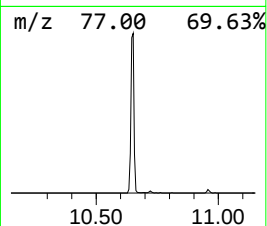
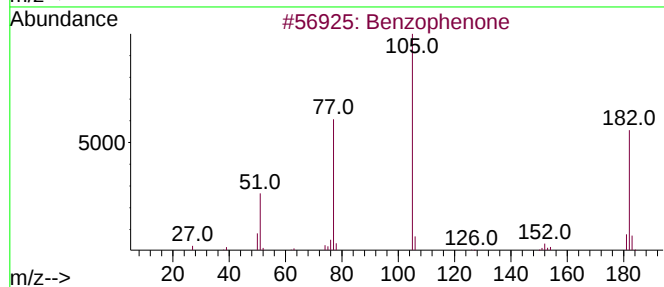
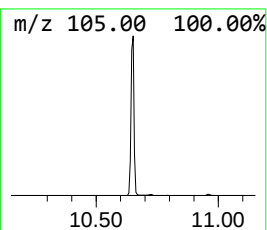
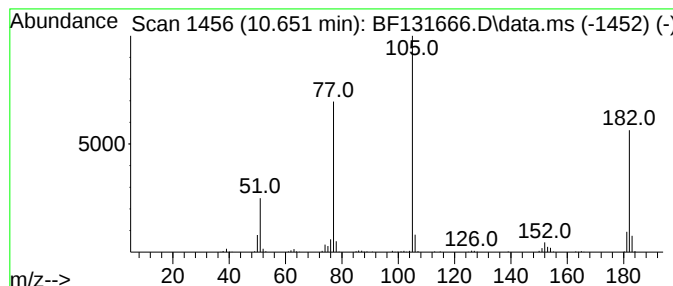
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.651	12.63 ng	384447	Acenaphthene-d10		9.934	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzophenone		182	C13H10O	000119-61-9	96
2	Azobenzene		182	C12H10N2	000103-33-3	64
3	N-Methoxy-N-methylbenzamide		165	C9H11NO2	006919-61-5	49
4	1-Propanone, 3-chloro-1-phenyl-		168	C9H9ClO	000936-59-4	47
5	1-Propanone, 2-bromo-1-phenyl-		212	C9H9BrO	002114-00-3	47



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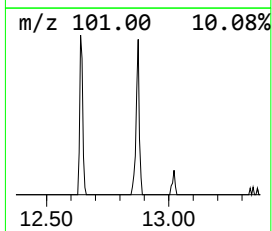
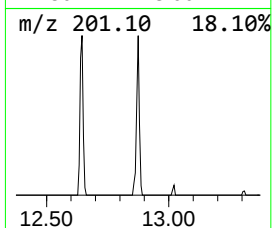
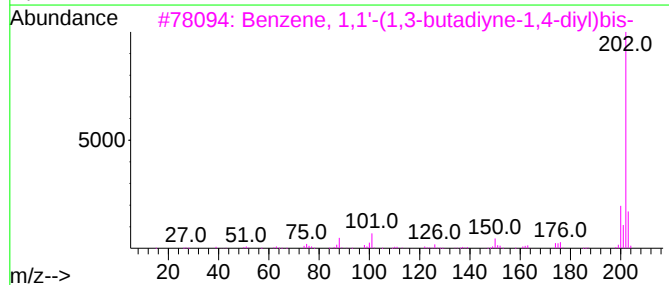
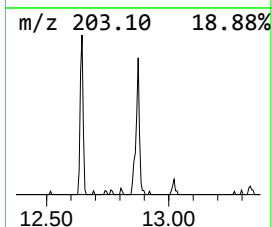
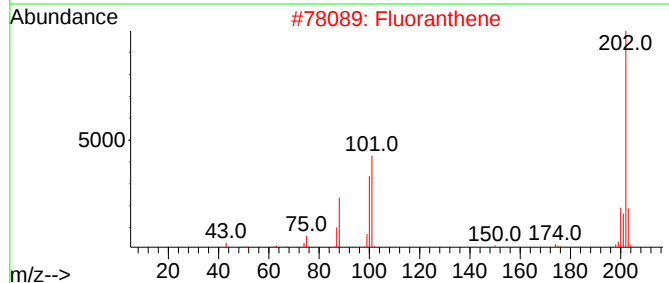
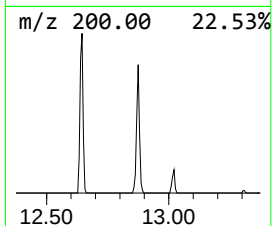
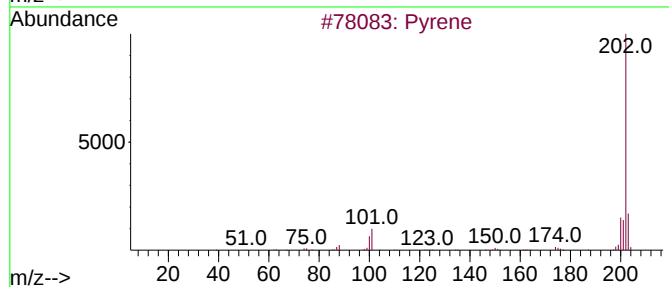
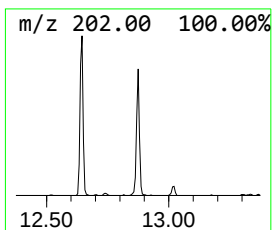
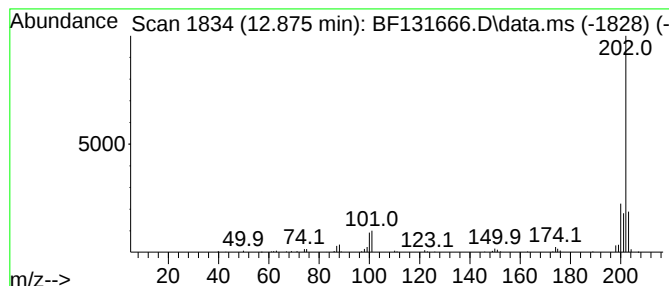
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.874	2.91 ng	78470	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene	202	C16H10	000129-00-0	96
2			Fluoranthene	202	C16H10	000206-44-0	87
3			Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	59
4			1-Leucyl-1-leucine, N,N'-dimethy...	528	C29H56N2O6	1000328-59-7	33
5			Benzaldehyde, 2,6-difuloro-3,4-d...	202	C9H8F2O3	152434-99-6	9



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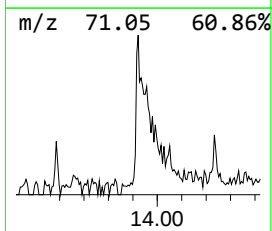
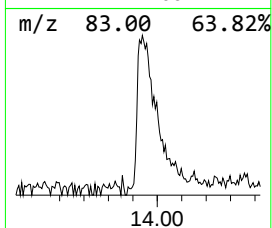
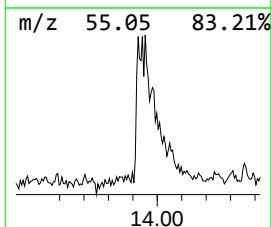
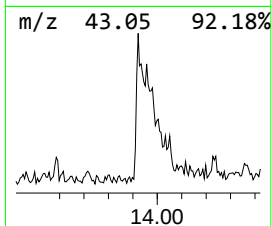
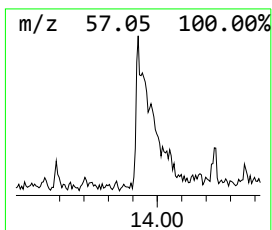
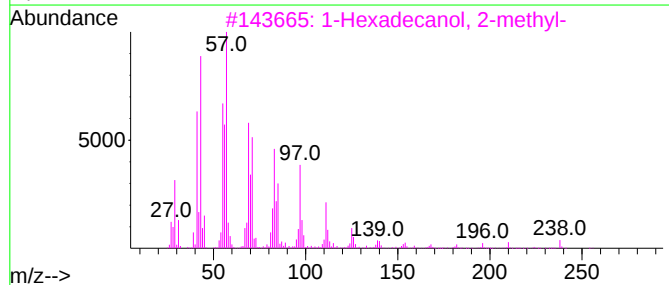
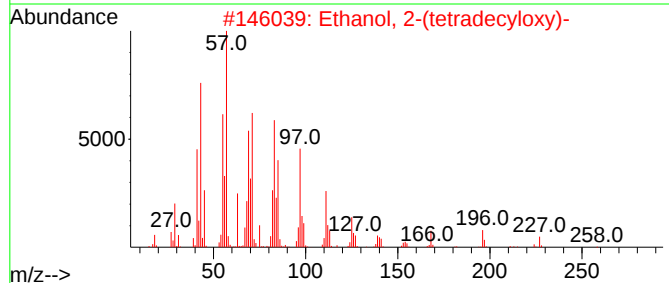
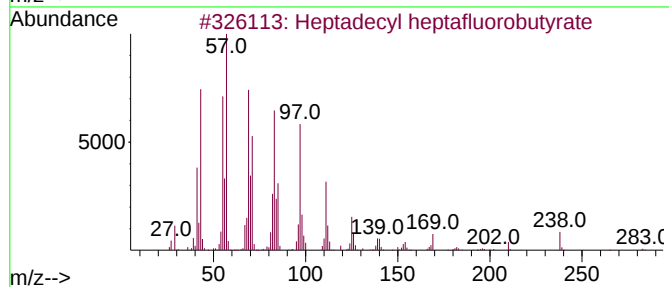
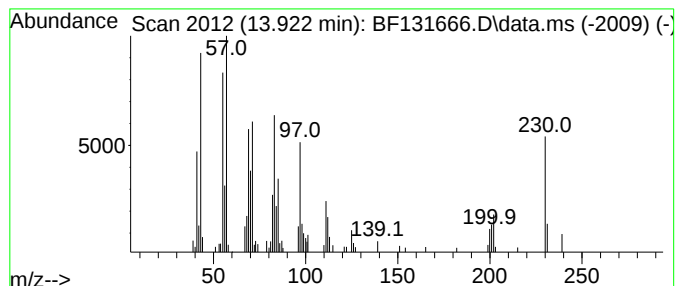
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Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.922	3.46 ng	93484	Chrysene-d12	14.080	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	76
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	76
3	1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	76
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	70
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	68



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ClientSampleId :
RB-37-(3-5)

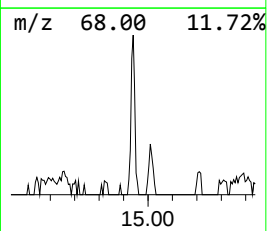
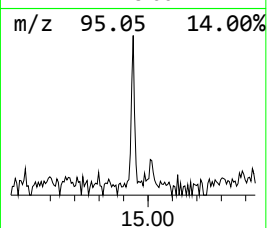
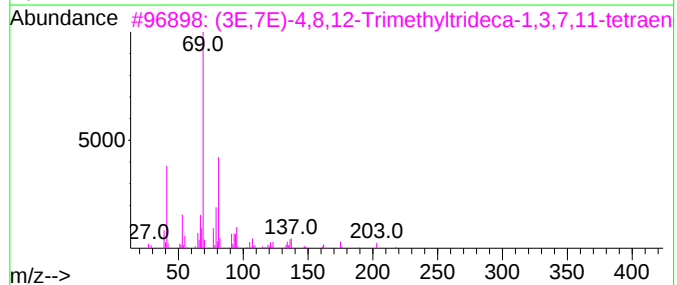
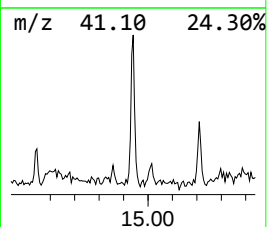
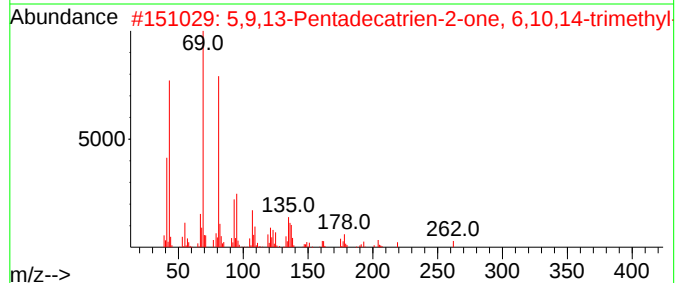
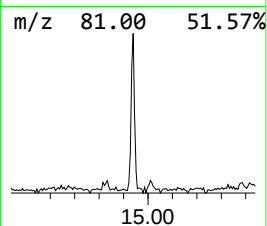
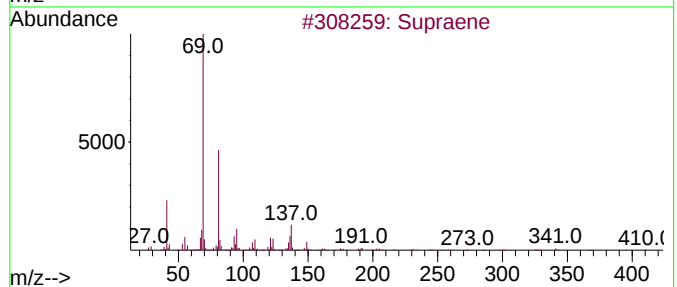
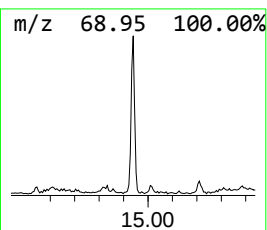
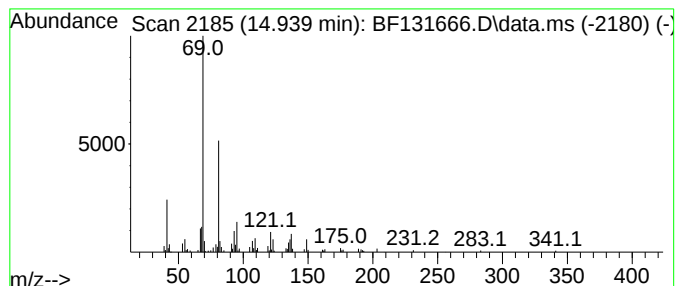
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.939	3.82 ng	79487	Perylene-d12	15.580

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Supraene	410	C30H50	007683-64-9	91
2		5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	64
3		(3E,7E)-4,8,12-Trimethyltrideca...	218	C16H26	062235-06-7	59
4		3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	59
5		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121622\
Data File : BF131666.D
Acq On : 16 Dec 2022 14:52
Operator : CG\JU
Sample : N6038-17
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-37-(3-5)

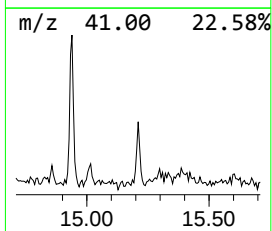
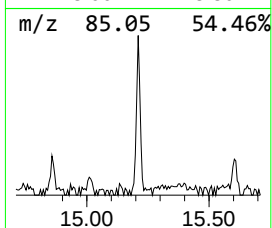
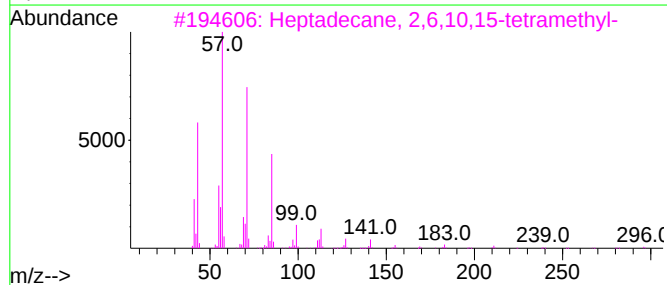
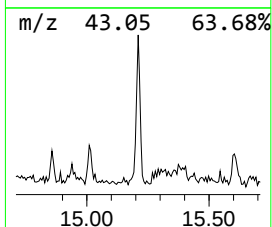
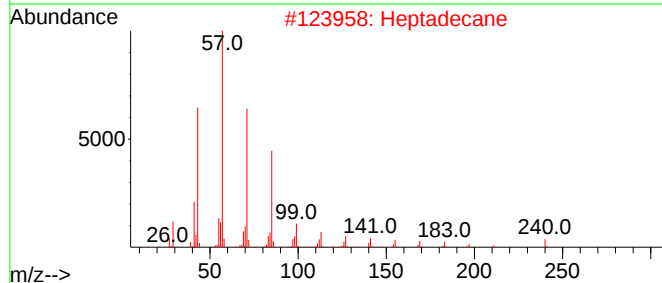
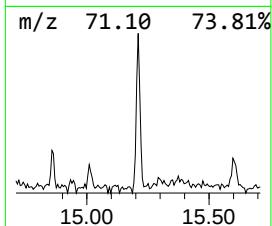
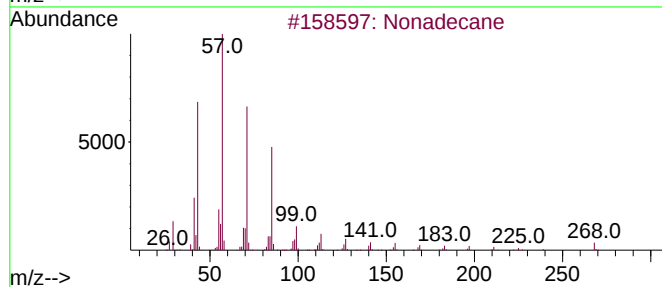
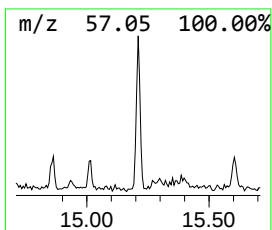
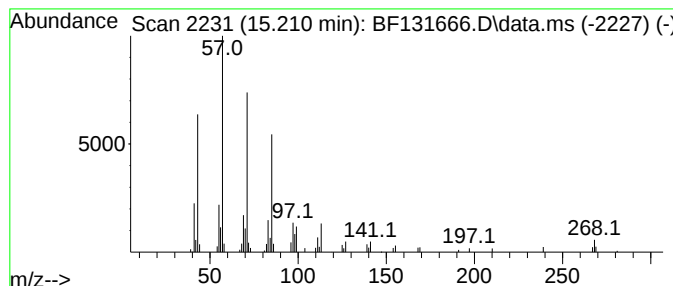
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.210	2.52 ng	52433	Perylene-d12	15.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	93
2			Heptadecane	240	C17H36	000629-78-7	86
3			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
4			Hexacosane	366	C26H54	000630-01-3	80
5			Tetratetracontane	619	C44H90	007098-22-8	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121622\
Data File : BF131666.D
Acq On : 16 Dec 2022 14:52
Operator : CG\JU
Sample : N6038-17
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-37-(3-5)

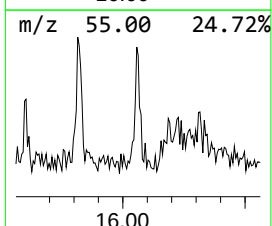
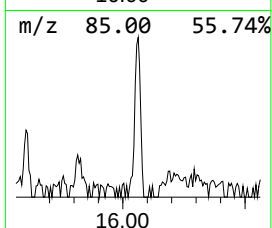
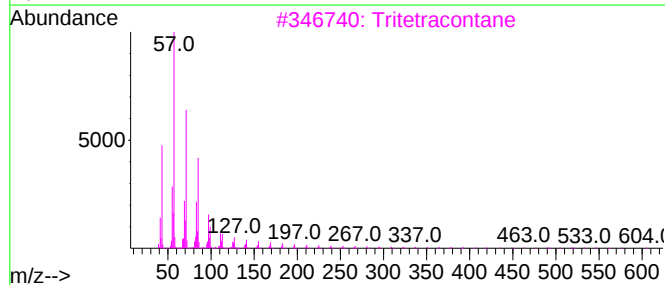
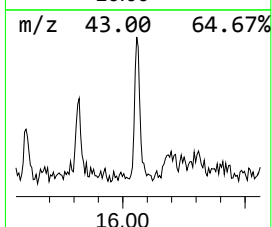
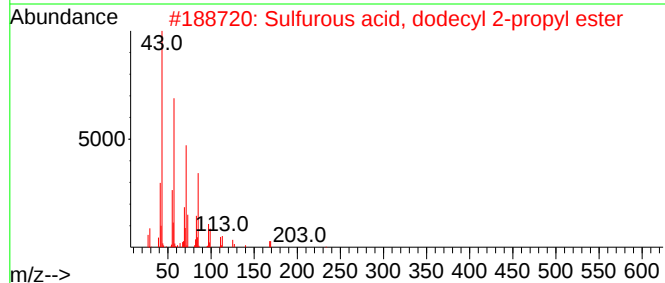
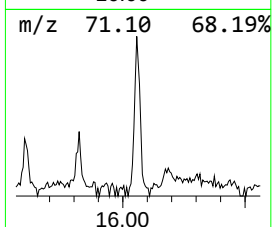
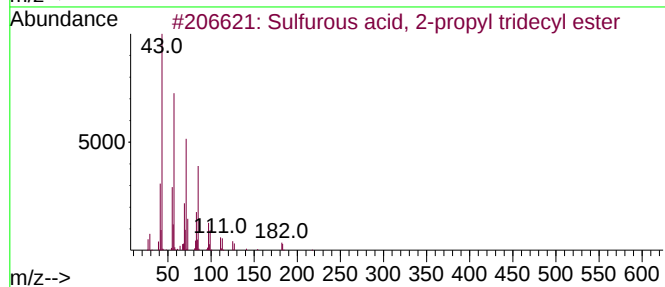
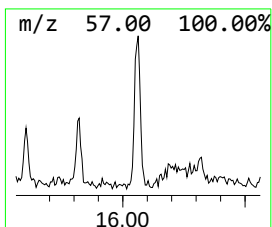
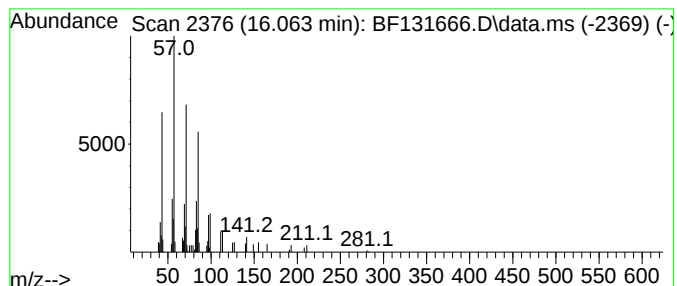
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Sulfurous acid, 2-propyl tr... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.063	2.28 ng	47426	Perylene-d12	15.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, 2-propyl tridecyl...	306	C16H34O3S	1000309-12-4	90
2			Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	90
3			Tritetracontane	605	C43H88	007098-21-7	90
4			Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	86
5			Nonadecane, 9-methyl-	282	C20H42	013287-24-6	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121622\
Data File : BF131666.D
Acq On : 16 Dec 2022 14:52
Operator : CG\JU
Sample : N6038-17
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-37-(3-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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...	2.134	17.0	ng	360282	1	6.881	424621	20.0
2-Pentanone, 4-...	5.087	12.6	ng	267944	1	6.881	424621	20.0
Benzophenone	10.651	12.6	ng	384447	3	9.934	608556	20.0
Benzene, 1,1'-(...	12.874	2.9	ng	78470	5	14.080	540023	20.0
Heptadecyl hept...	13.922	3.5	ng	93484	5	14.080	540023	20.0
Supraene	14.939	3.8	ng	79487	6	15.580	416546	20.0
Nonadecane	15.210	2.5	ng	52433	6	15.580	416546	20.0
Sulfurous acid,...	16.063	2.3	ng	47426	6	15.580	416546	20.0