

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112322\
 Data File : BF131376.D
 Acq On : 23 Nov 2022 23:16
 Operator : CG\JU
 Sample : N5642-07
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RIGHT-SIDE-FLATS-27

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-BF112122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131376.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.316	30	39	45	rVB	962491	1254279	47.95%	6.440%
2	5.187	522	527	534	rBV	339492	425475	16.27%	2.185%
3	5.569	587	592	595	rBV	2522742	2615741	100.00%	13.430%
4	6.569	756	762	765	rBV	2350999	2581921	98.71%	13.257%
5	6.951	823	827	831	rVB	828850	656937	25.11%	3.373%
6	7.516	917	923	926	rBV	1654075	1647689	62.99%	8.460%
7	8.239	1041	1046	1050	rBV	961874	799958	30.58%	4.107%
8	9.322	1224	1230	1233	rBV	3133965	2604802	99.58%	13.374%
9	10.004	1341	1346	1350	rBV	984672	805911	30.81%	4.138%
10	10.721	1463	1468	1471	rBV	376204	285709	10.92%	1.467%
11	10.798	1476	1481	1484	rBV	1549353	1396486	53.39%	7.170%
12	11.498	1596	1600	1604	rBV	787360	675802	25.84%	3.470%
13	11.604	1614	1618	1620	rVB	42057	31233	1.19%	0.160%
14	12.021	1684	1689	1694	rBV	170991	162181	6.20%	0.833%
15	12.810	1818	1823	1828	rBV	43007	45093	1.72%	0.232%
16	13.098	1867	1872	1875	rBV	2068675	1851128	70.77%	9.504%
17	13.998	2022	2025	2027	rBV2	42210	48491	1.85%	0.249%
18	14.157	2048	2052	2055	rBV	673102	546564	20.90%	2.806%
19	14.251	2063	2068	2073	rBV	92790	113173	4.33%	0.581%
20	14.315	2076	2079	2085	rVB	35585	34521	1.32%	0.177%
21	14.627	2129	2132	2137	rVB	41739	42774	1.64%	0.220%
22	14.951	2185	2187	2191	rVB	41378	41903	1.60%	0.215%
23	15.033	2198	2201	2205	rBV2	49514	55166	2.11%	0.283%
24	15.315	2246	2249	2256	rVB	50801	59524	2.28%	0.306%
25	15.692	2308	2313	2317	rBV	362906	463173	17.71%	2.378%
26	15.727	2317	2319	2323	rVB2	49466	58741	2.25%	0.302%
27	16.203	2395	2400	2404	rBV	48175	70308	2.69%	0.361%
28	16.756	2489	2494	2500	rVB3	33103	62908	2.40%	0.323%
29	17.403	2600	2604	2609	rVB3	22717	39023	1.49%	0.200%

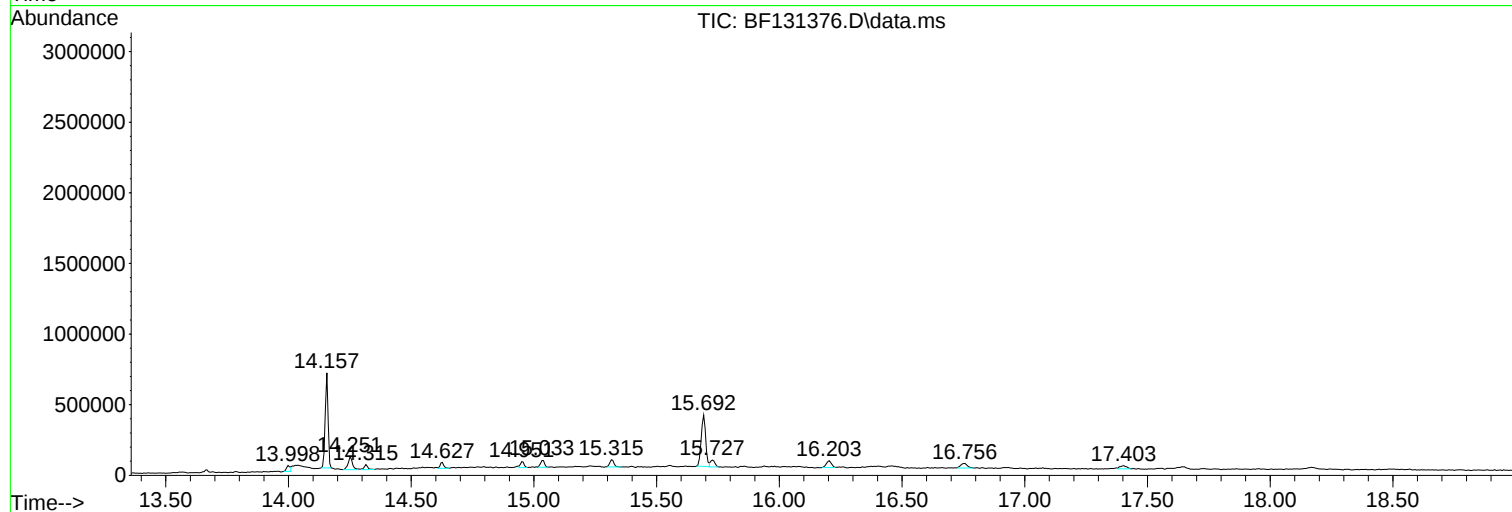
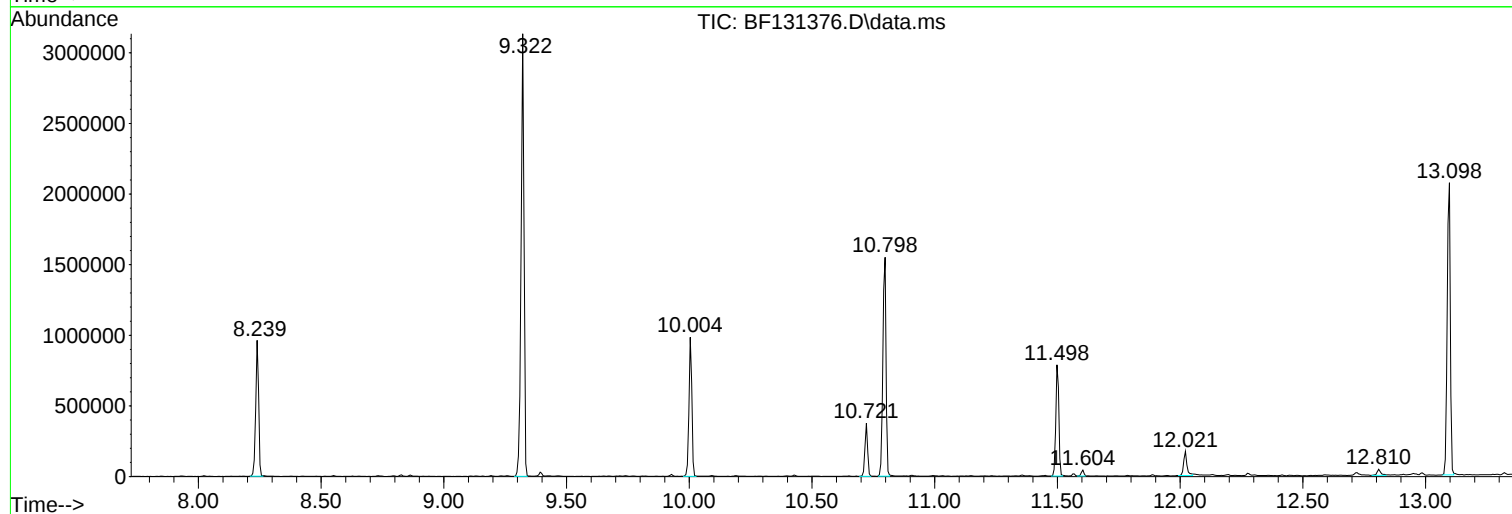
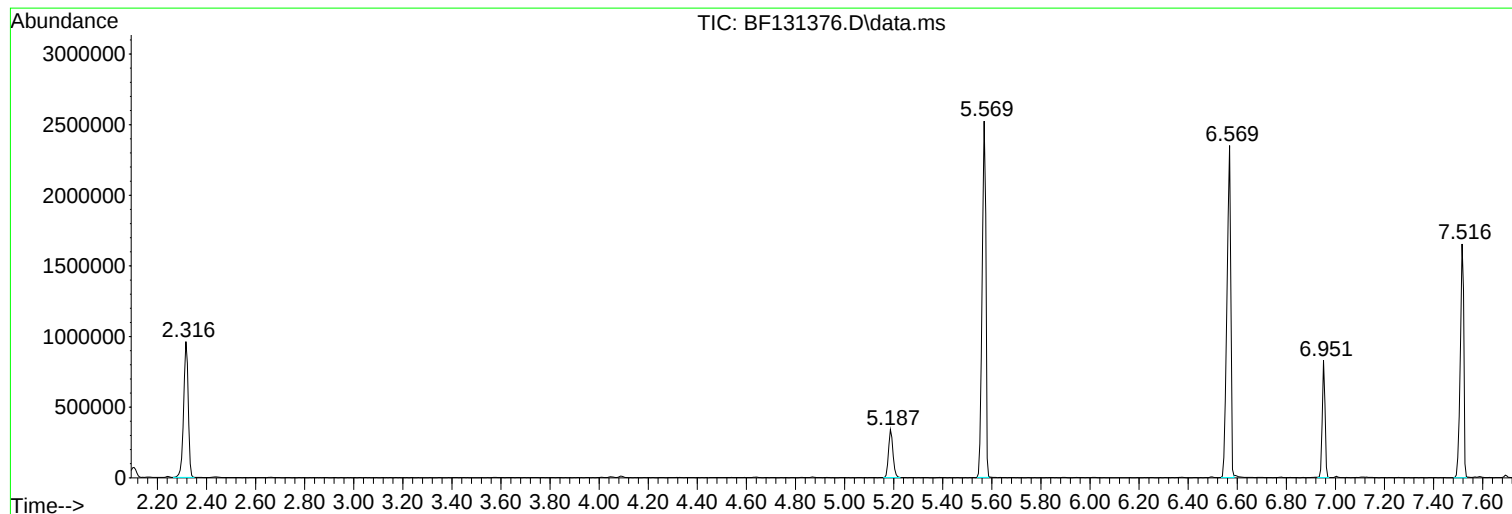
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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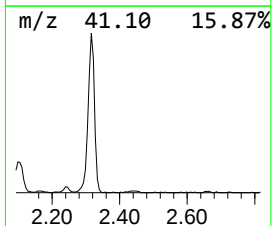
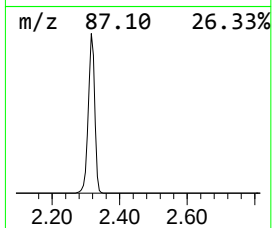
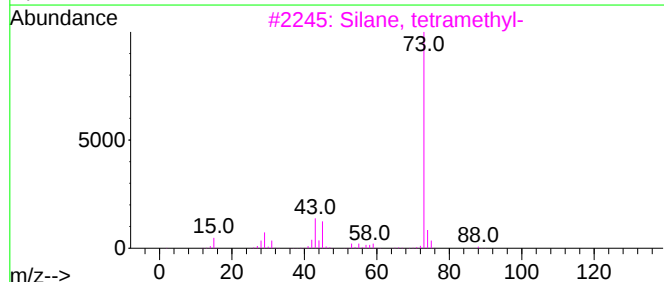
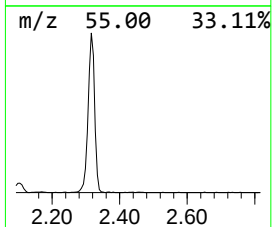
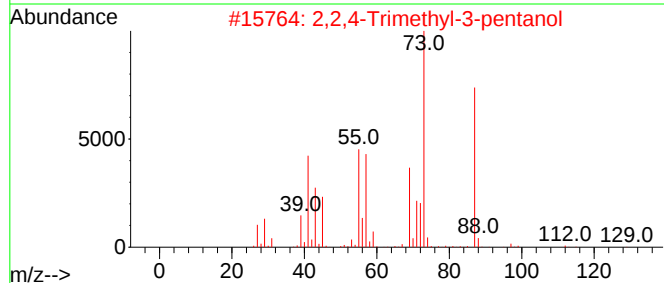
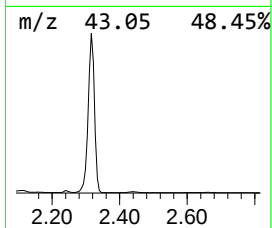
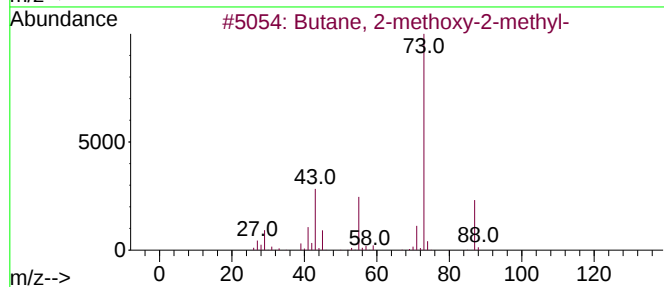
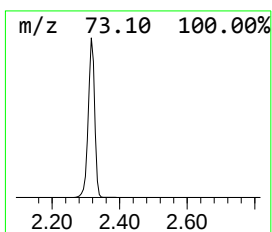
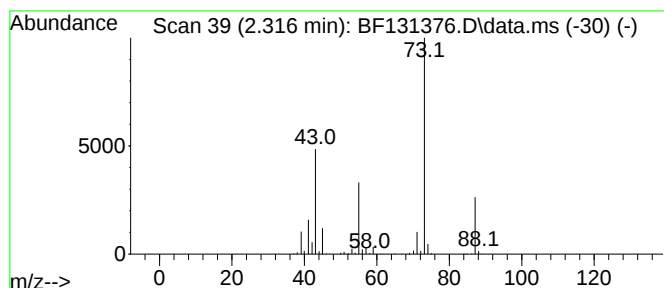
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.316	38.19 ng	1254280	1,4-Dichlorobenzene-d4	6.951

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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	23
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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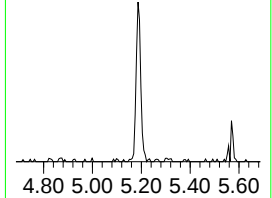
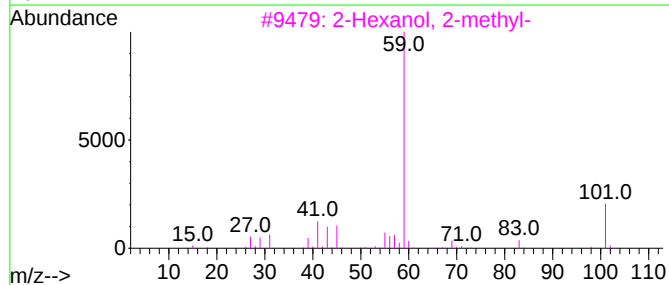
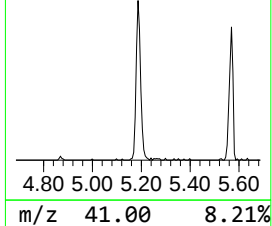
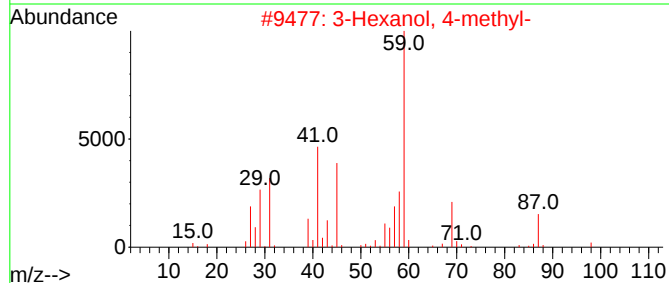
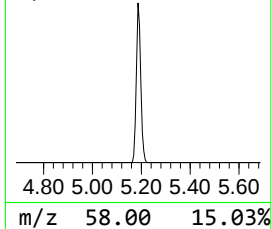
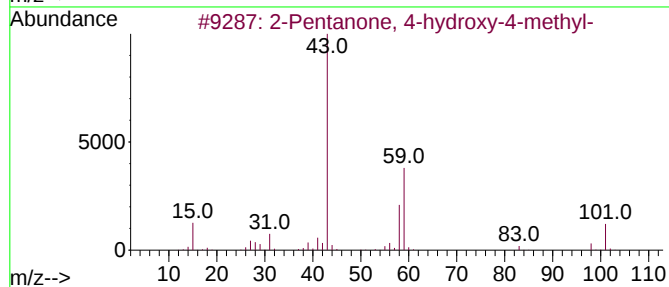
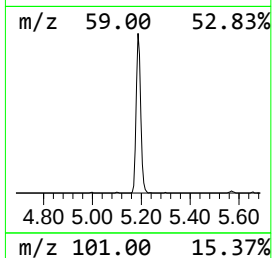
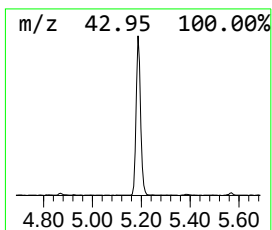
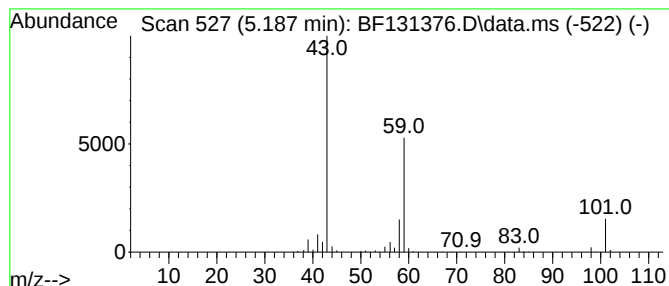
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.187	12.95 ng	425475	1,4-Dichlorobenzene-d4	6.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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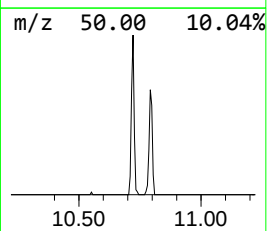
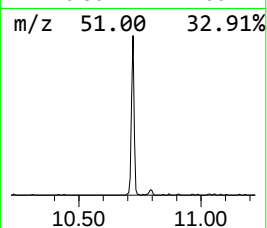
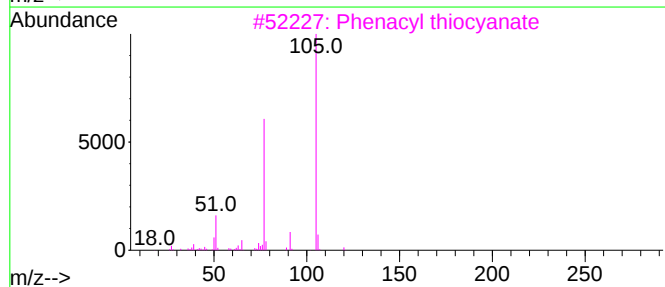
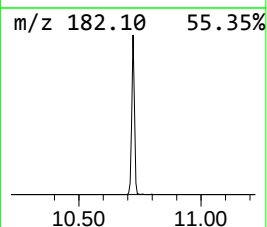
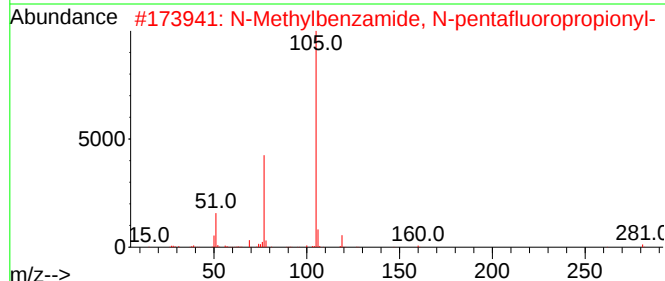
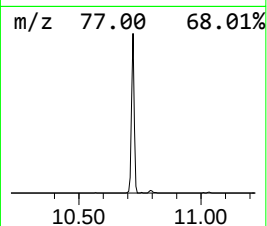
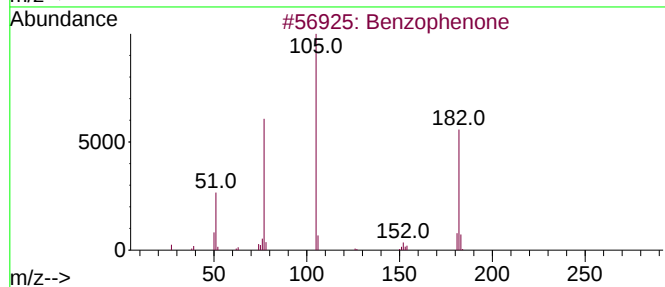
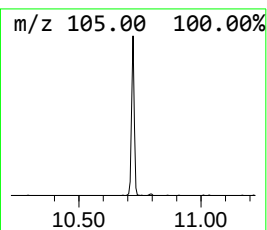
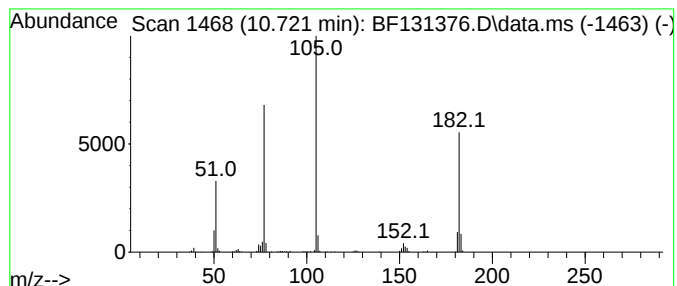
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Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.722	7.09 ng	285709	Acenaphthene-d10	10.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	47
3			Phenacyl thiocyanate	177	C9H7NOS	005399-30-4	47
4			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
5			Benzoylformic acid	150	C8H6O3	000611-73-4	47



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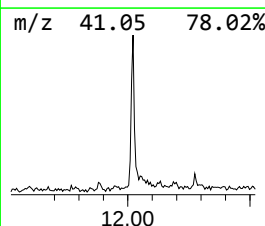
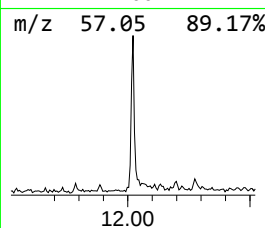
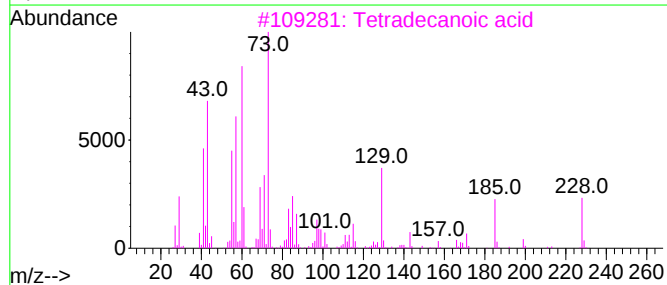
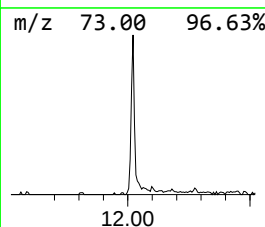
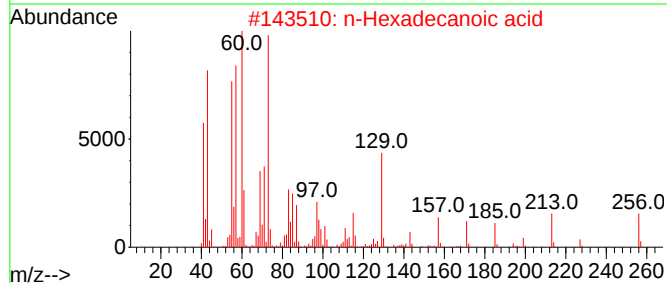
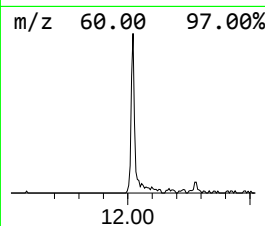
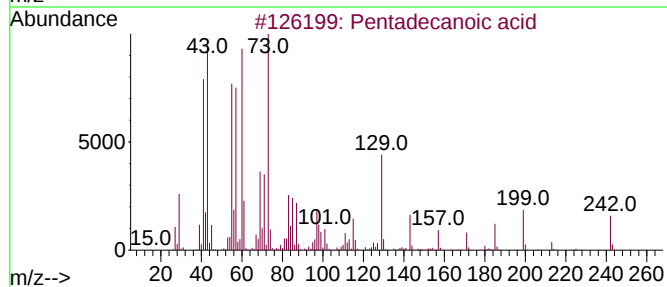
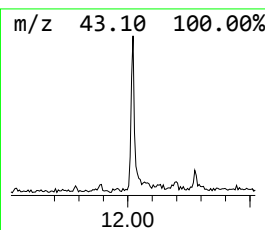
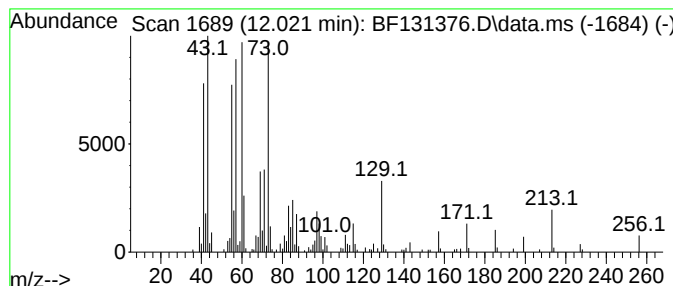
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Peak Number 4 Pentadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.021	4.80 ng	162181	Phenanthrene-d10	11.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	70
5			Undecanoic acid	186	C11H22O2	000112-37-8	68



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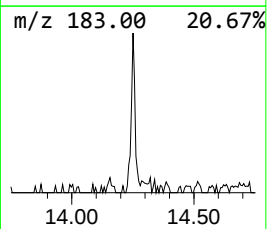
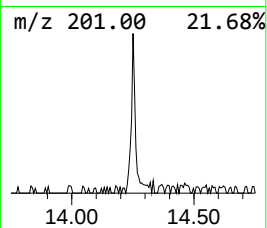
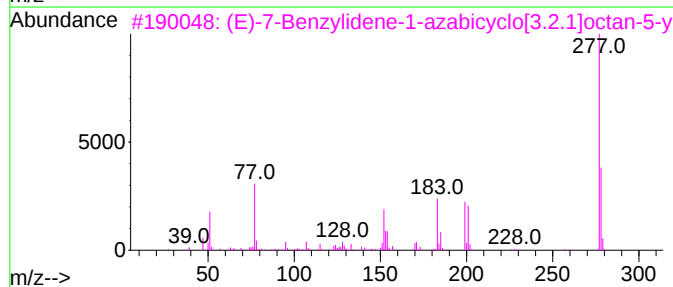
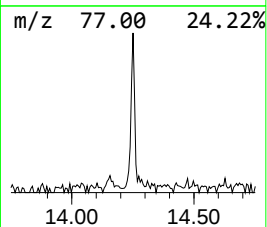
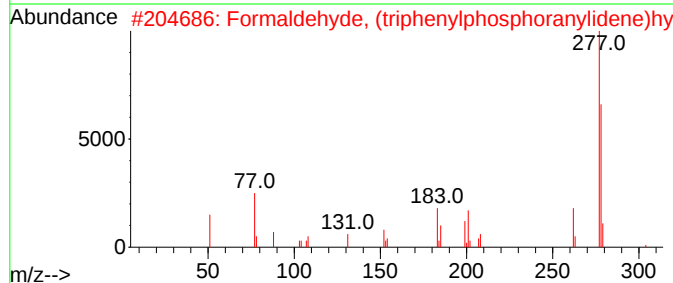
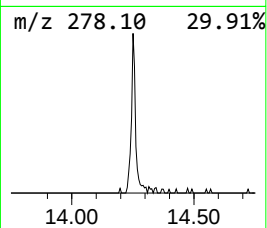
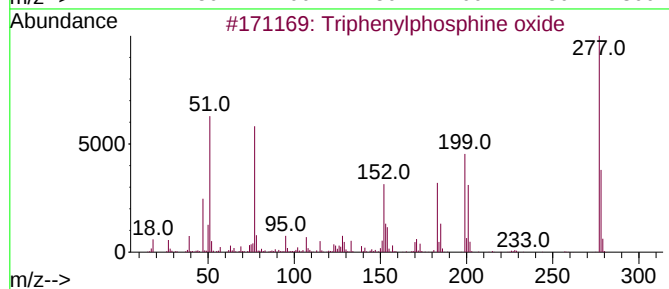
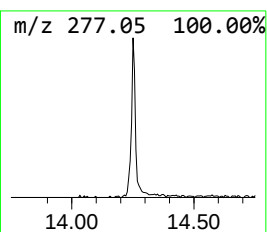
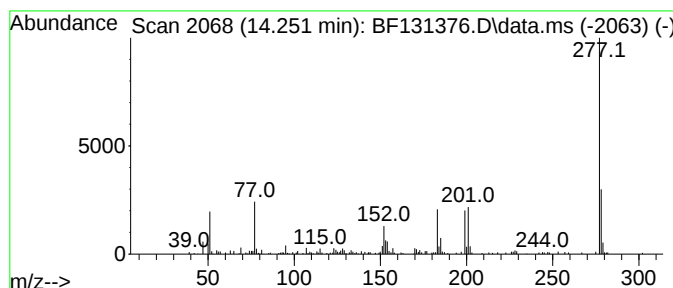
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.251	4.14 ng	113173	Chrysene-d12	14.156

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	72
3			(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19N03S	1000483-83-4	64
4			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	38
5			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	32



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RIGHT-SIDE-FLATS-27

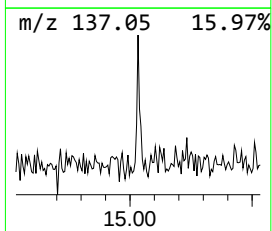
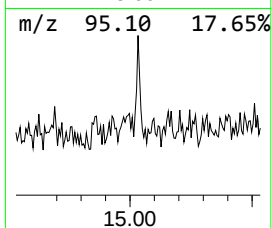
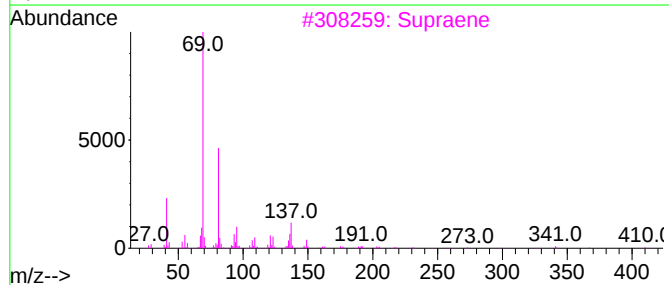
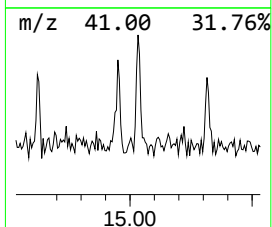
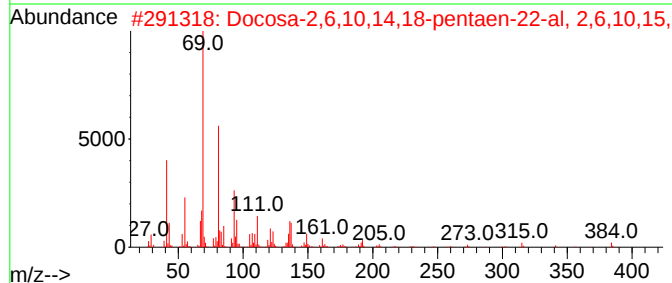
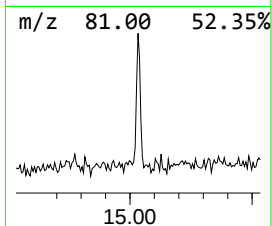
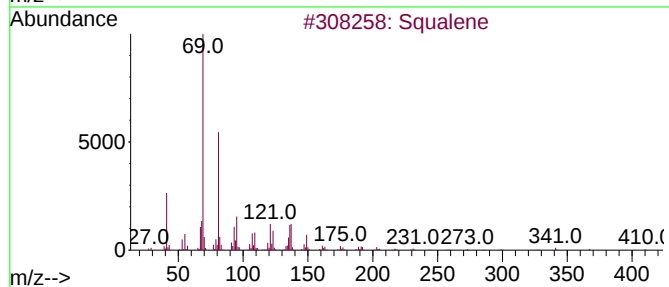
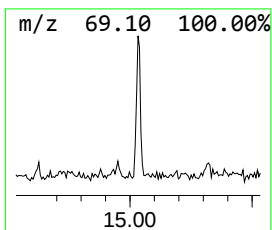
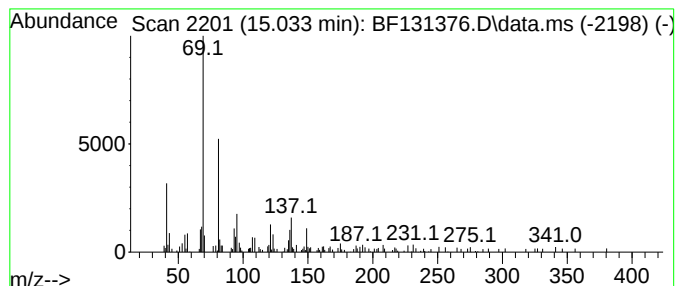
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.033	2.38 ng	55166	Perylene-d12	15.692

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Squalene	410	C30H50	000111-02-4	87
2		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	86
3		Supraene	410	C30H50	007683-64-9	86
4		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
5		trans-Farnesol	222	C15H26O	000106-28-5	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112322\
Data File : BF131376.D
Acq On : 23 Nov 2022 23:16
Operator : CG\JU
Sample : N5642-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RIGHT-SIDE-FLATS-27

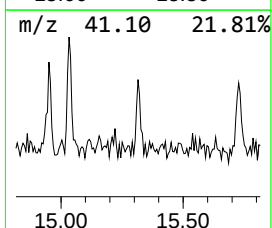
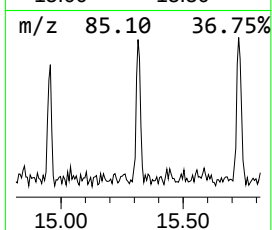
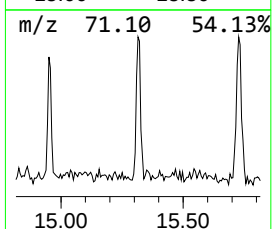
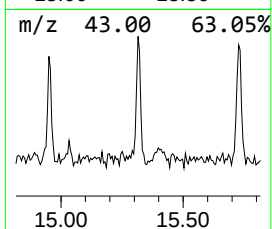
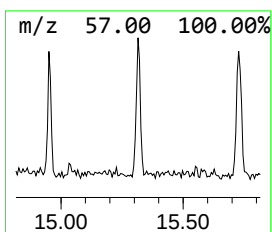
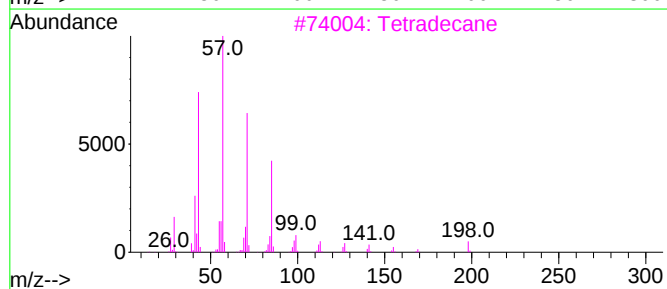
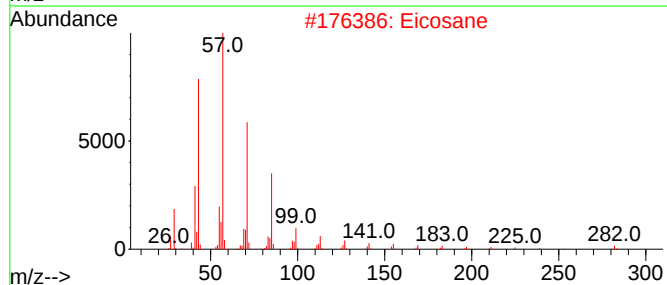
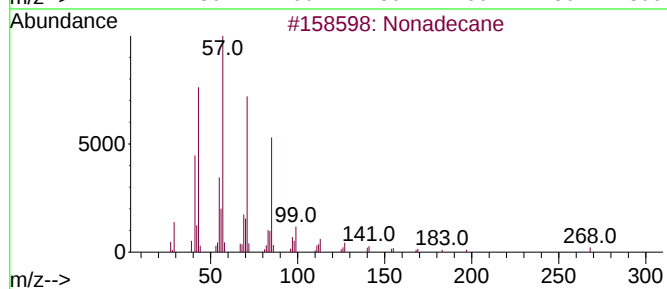
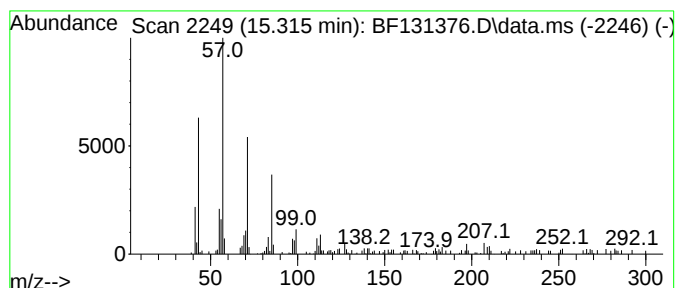
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.315	2.57 ng	59524	Perylene-d12	15.692

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	93
2			Eicosane	282	C20H42	000112-95-8	87
3			Tetradecane	198	C14H30	000629-59-4	81
4			Octadecane	254	C18H38	000593-45-3	74
5			Heneicosane	296	C21H44	000629-94-7	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112322\
Data File : BF131376.D
Acq On : 23 Nov 2022 23:16
Operator : CG\JU
Sample : N5642-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

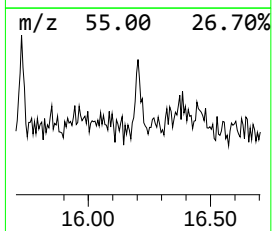
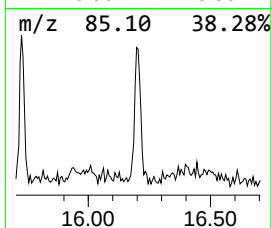
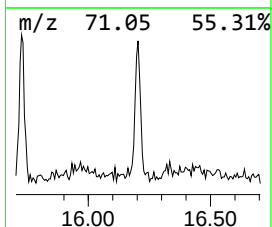
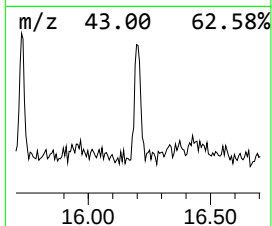
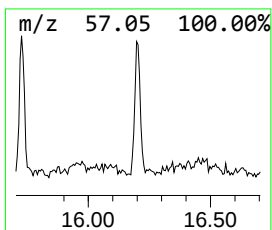
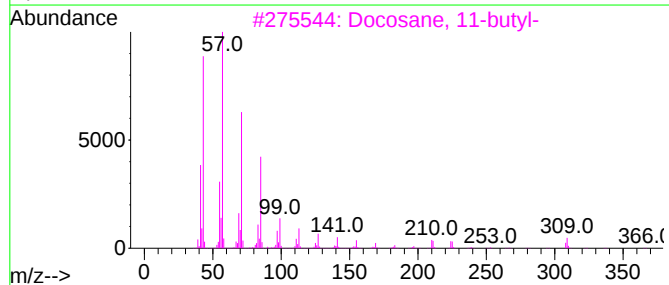
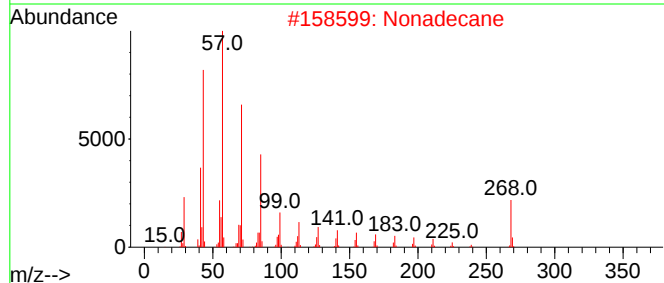
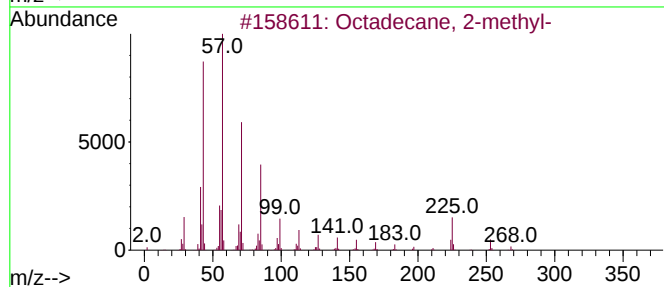
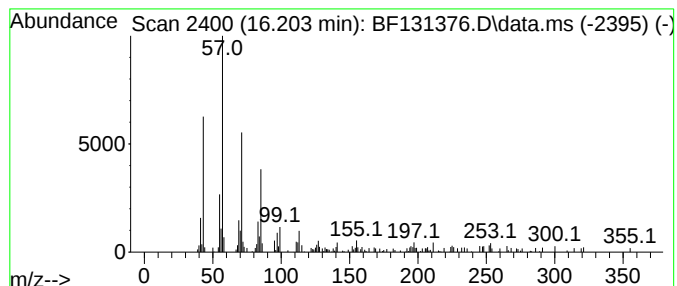
Instrument :
BNA_F
ClientSampleId :
RIGHT-SIDE-FLATS-27

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.203	3.04 ng	70308	Perylene-d12	15.692	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
2	Nonadecane	268	C19H40	000629-92-5	90
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	90
4	Pentacosane	352	C25H52	000629-99-2	90
5	Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112322\
Data File : BF131376.D
Acq On : 23 Nov 2022 23:16
Operator : CG\JU
Sample : N5642-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RIGHT-SIDE-FLATS-27

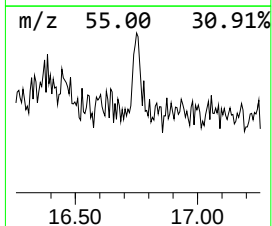
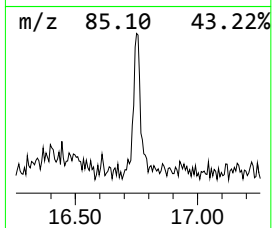
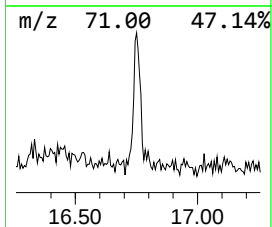
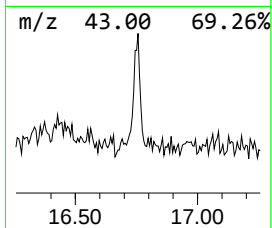
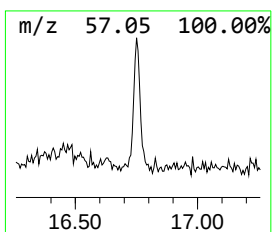
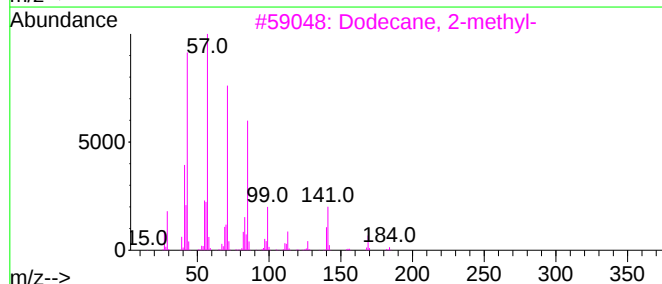
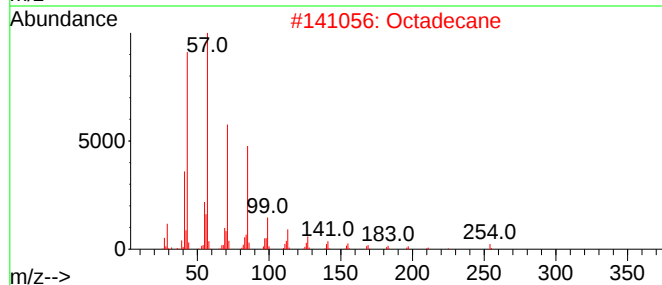
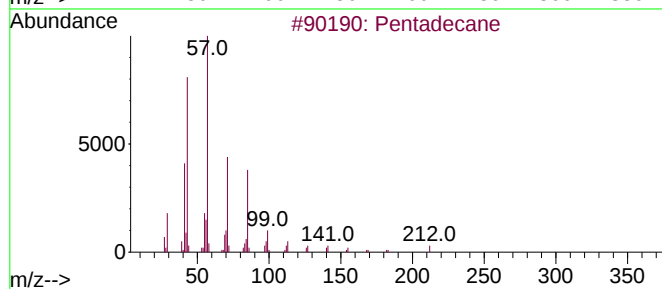
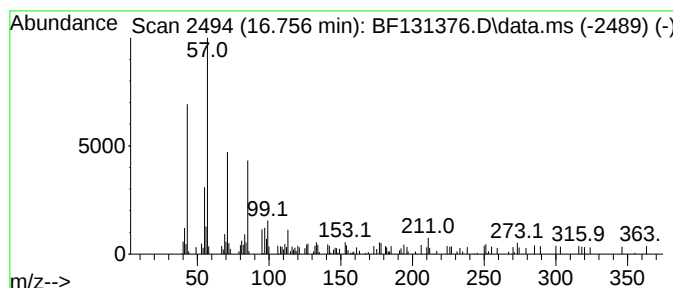
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.756	2.72 ng	62908	Perylene-d12	15.692

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane	212	C15H32	000629-62-9	83
2			Octadecane	254	C18H38	000593-45-3	58
3			Dodecane, 2-methyl-	184	C13H28	001560-97-0	58
4			Heneicosane	296	C21H44	000629-94-7	58
5			Heptadecane	240	C17H36	000629-78-7	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112322\
Data File : BF131376.D
Acq On : 23 Nov 2022 23:16
Operator : CG\JU
Sample : N5642-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RIGHT-SIDE-FLATS-27

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.316	38.2	ng	1254280	1	6.951	656937	20.0
2-Pentanone, 4-...	5.187	12.9	ng	425475	1	6.951	656937	20.0
Benzophenone	10.722	7.1	ng	285709	3	10.004	805911	20.0
Pentadecanoic acid	12.021	4.8	ng	162181	4	11.498	675802	20.0
Triphenylphosph...	14.251	4.1	ng	113173	5	14.156	546564	20.0
Squalene	15.033	2.4	ng	55166	6	15.692	463173	20.0
Nonadecane	15.315	2.6	ng	59524	6	15.692	463173	20.0
Octadecane, 2-m...	16.203	3.0	ng	70308	6	15.692	463173	20.0
Pentadecane	16.756	2.7	ng	62908	6	15.692	463173	20.0