

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112322\
 Data File : BF131382.D
 Acq On : 24 Nov 2022 02:28
 Operator : CG\JU
 Sample : N5642-06
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RIGHT-SIDE-FLATS-26

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: BF131382.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.299	28	36	42	rVB	883284	1144290	47.89%	6.308%
2	5.187	522	527	534	rVB	308754	389713	16.31%	2.148%
3	5.569	587	592	595	rBV	2484835	2389210	100.00%	13.170%
4	6.569	756	762	765	rBV	2193006	2373440	99.34%	13.084%
5	6.957	824	828	831	rVB	778042	706024	29.55%	3.892%
6	7.522	916	924	927	rBV	1444218	1444541	60.46%	7.963%
7	8.245	1042	1047	1050	rBV	883067	815766	34.14%	4.497%
8	9.322	1225	1230	1233	rBV	2762676	2241978	93.84%	12.359%
9	10.010	1342	1347	1350	rBV	864858	782403	32.75%	4.313%
10	10.722	1464	1468	1474	rBV	74494	58304	2.44%	0.321%
11	10.798	1477	1481	1484	rBV	1386421	1196344	50.07%	6.595%
12	11.504	1597	1601	1604	rBV	802270	668733	27.99%	3.686%
13	12.021	1685	1689	1694	rBV	152921	135174	5.66%	0.745%
14	12.810	1819	1823	1828	rBV2	32503	37248	1.56%	0.205%
15	13.098	1868	1872	1875	rBV	2128620	1781073	74.55%	9.818%
16	14.033	2022	2031	2046	rBV8	65459	377968	15.82%	2.084%
17	14.157	2049	2052	2056	rVB	676493	606467	25.38%	3.343%
18	14.257	2064	2069	2074	rBV	125503	147549	6.18%	0.813%
19	14.321	2076	2080	2084	rVB	28577	35381	1.48%	0.195%
20	14.627	2129	2132	2135	rVB	44505	42526	1.78%	0.234%
21	14.957	2185	2188	2191	rVB	34480	36093	1.51%	0.199%
22	15.039	2199	2202	2209	rVB	52839	60839	2.55%	0.335%
23	15.321	2246	2250	2254	rBV	38982	50875	2.13%	0.280%
24	15.698	2309	2314	2318	rBV	348971	451622	18.90%	2.490%
25	15.733	2318	2320	2327	rVB	46419	56075	2.35%	0.309%
26	16.203	2397	2400	2407	rVB2	42410	64755	2.71%	0.357%
27	16.756	2491	2494	2499	rVB4	27931	46316	1.94%	0.255%

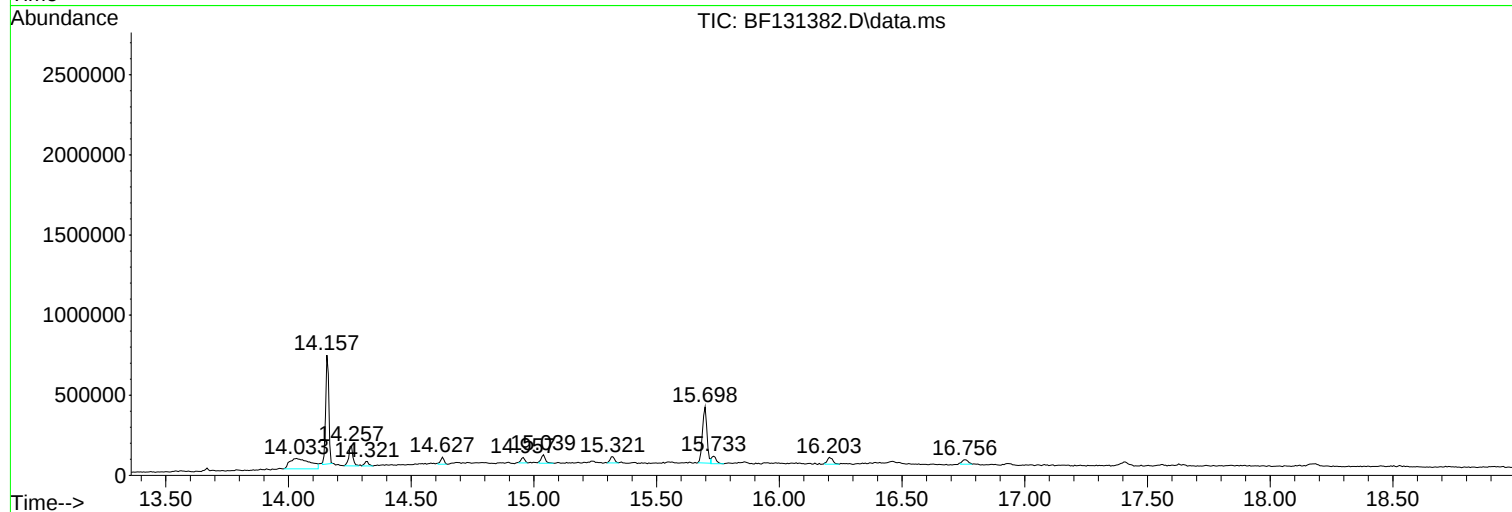
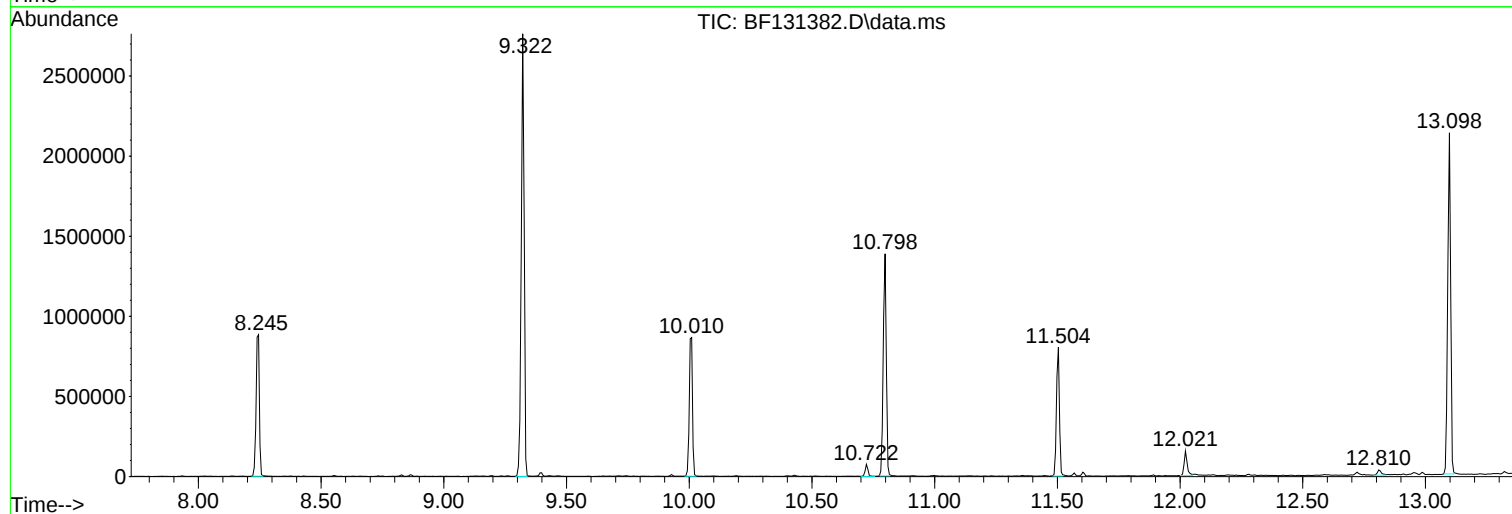
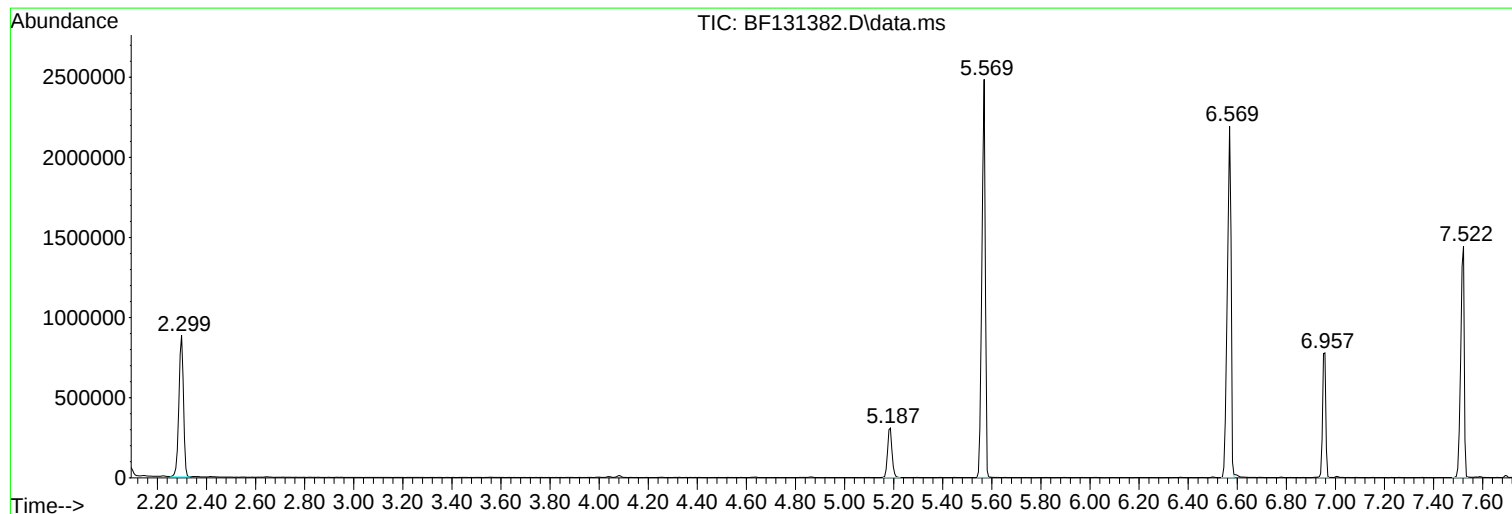
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Instrument :
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ClientSampleId :
RIGHT-SIDE-FLATS-26

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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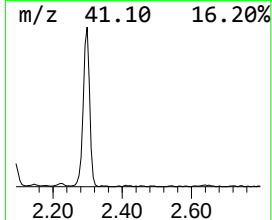
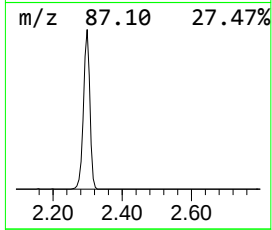
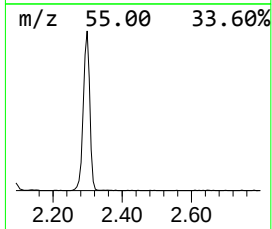
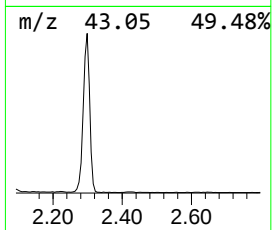
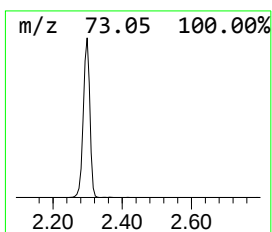
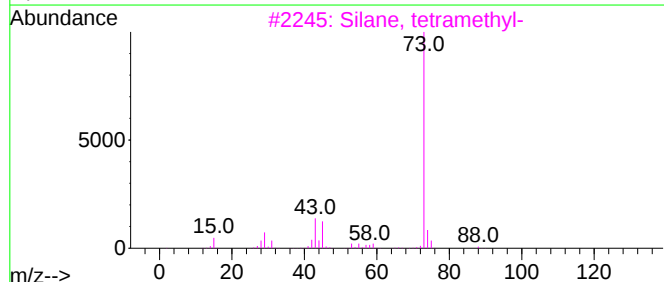
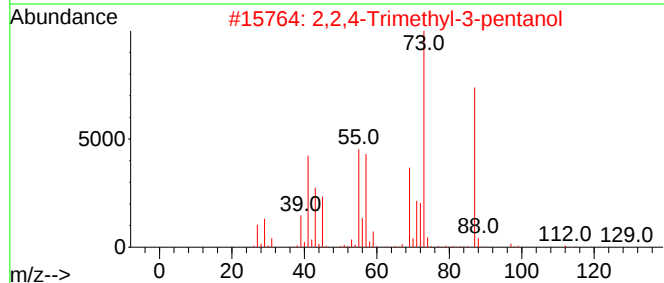
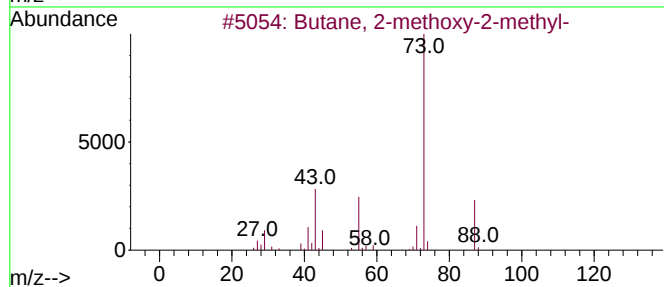
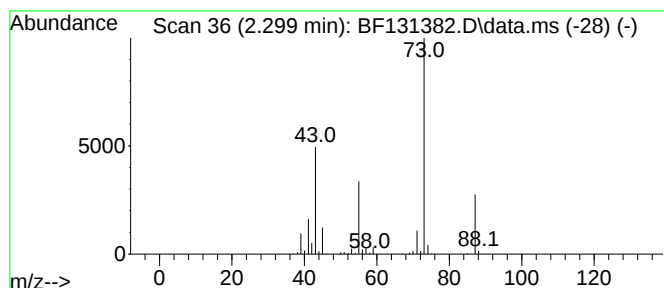
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.299	32.41 ng	1144290	1,4-Dichlorobenzene-d4	6.957

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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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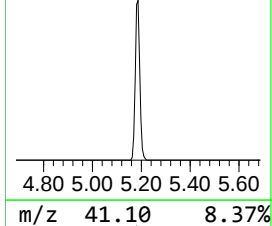
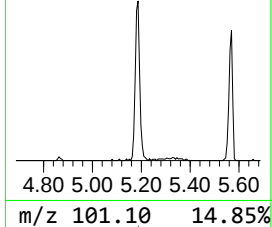
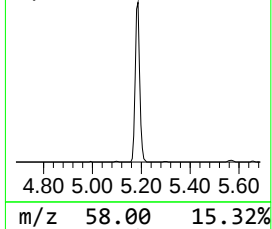
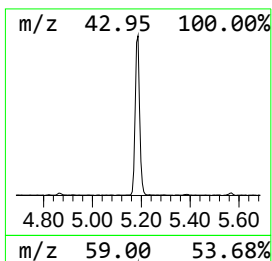
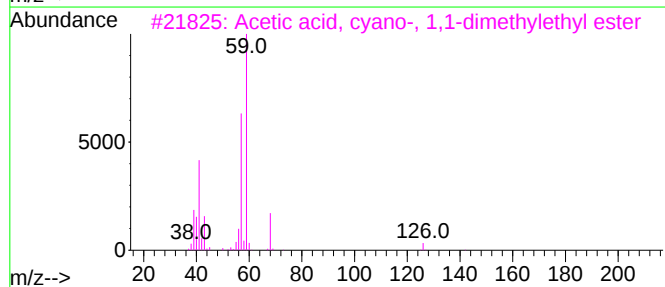
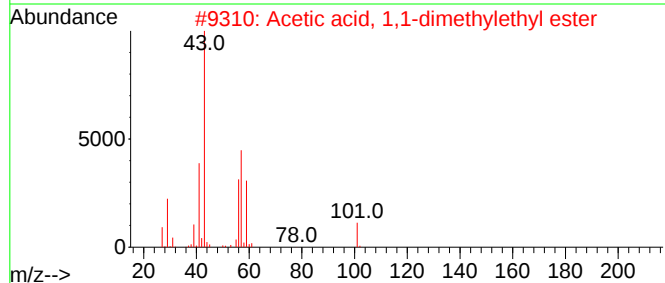
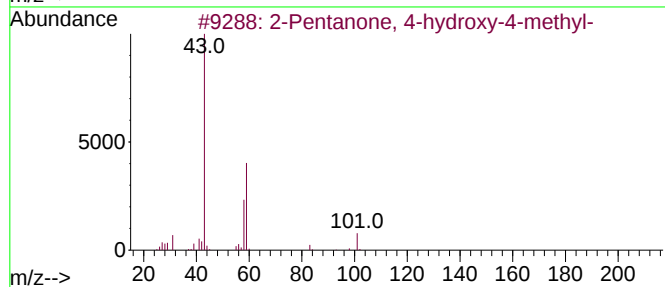
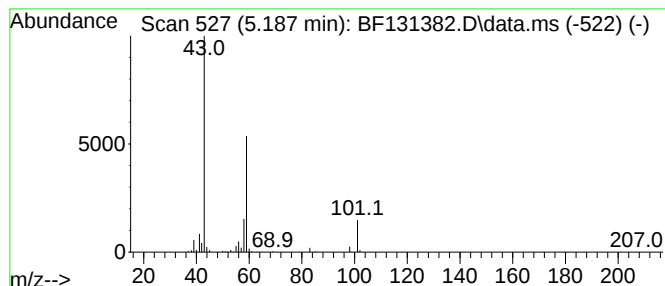
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.187	11.04 ng	389713	1,4-Dichlorobenzene-d4	6.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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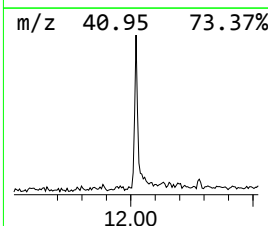
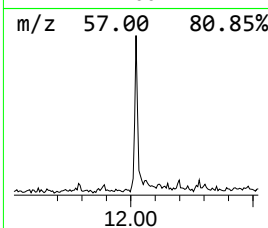
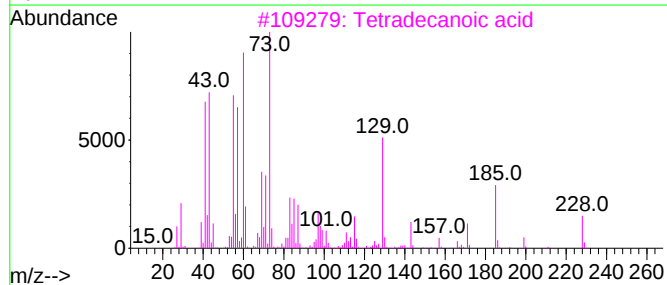
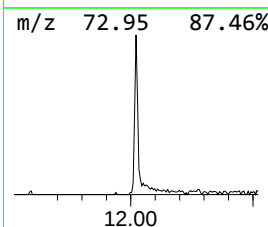
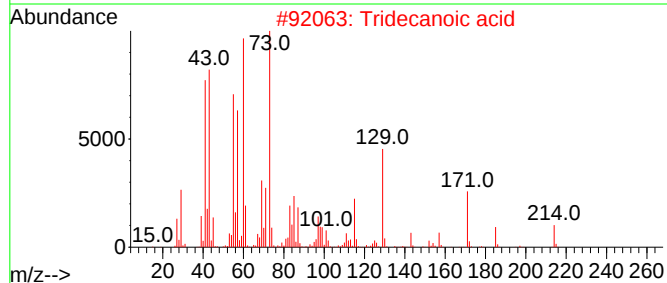
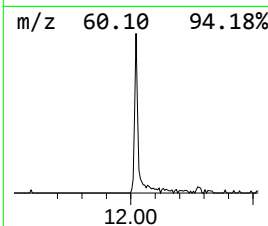
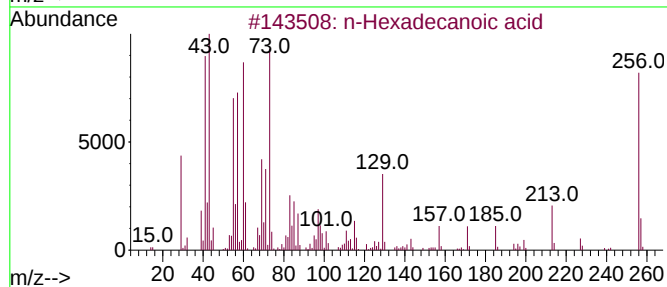
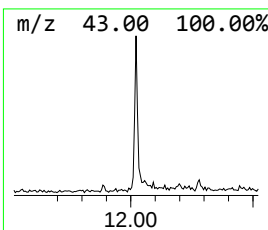
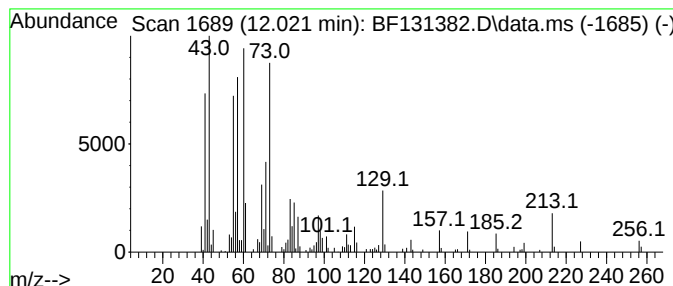
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.021	4.04 ng	135174	Phenanthrene-d10	11.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	92
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	70



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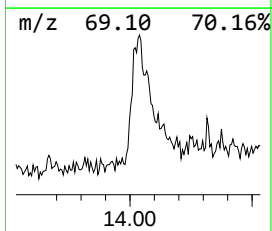
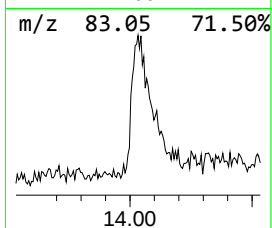
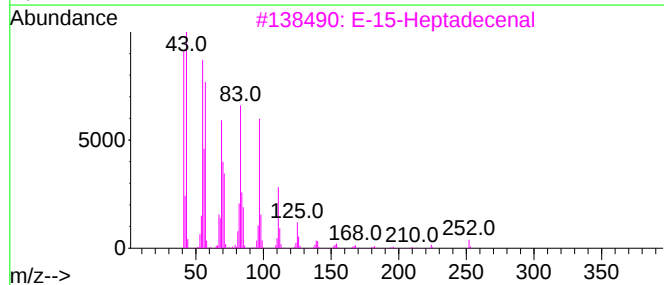
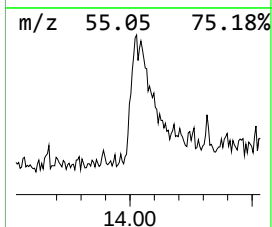
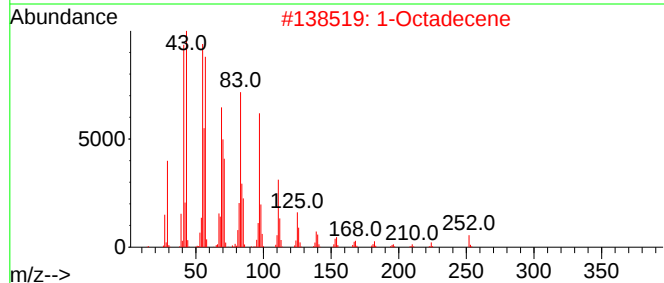
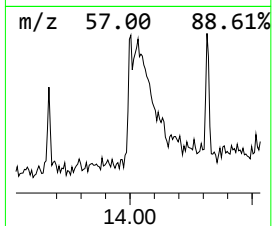
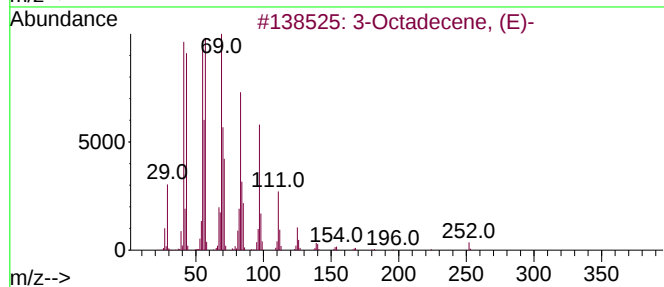
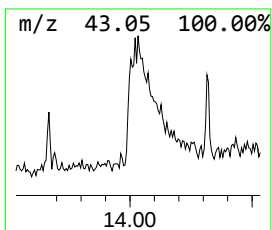
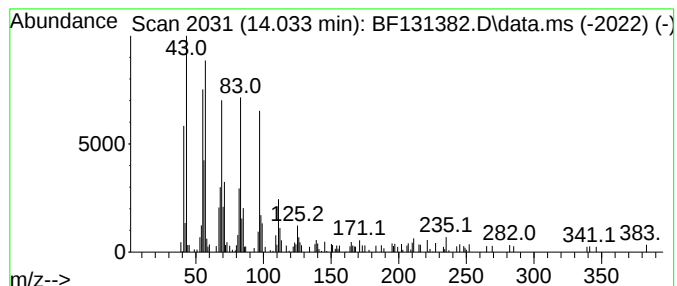
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Peak Number 4 3-Octadecene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.033	12.46 ng	377968	Chrysene-d12	14.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Octadecene, (E)-	252	C18H36	007206-19-1	93
2			1-Octadecene	252	C18H36	000112-88-9	93
3			E-15-Heptadecenal	252	C17H32O	1000130-97-9	93
4			1-Pentadecene	210	C15H30	013360-61-7	91
5			Pentafluoropropionic acid, dodec...	332	C15H25F5O2	006222-04-4	87



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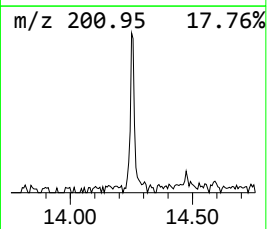
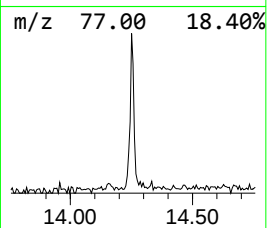
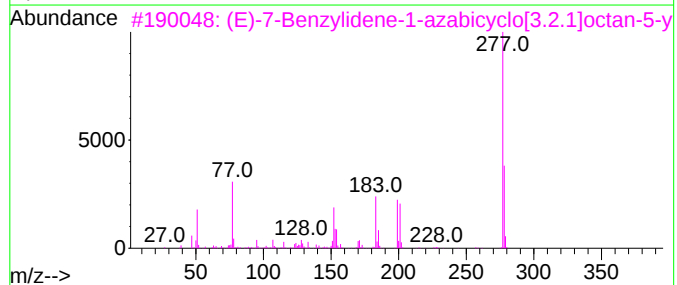
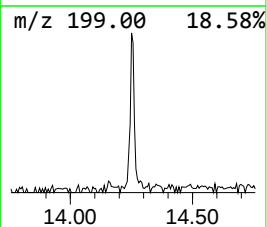
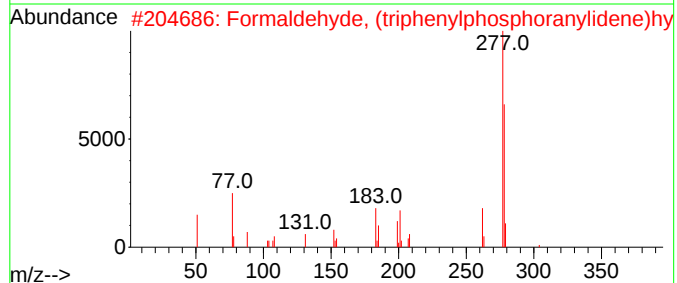
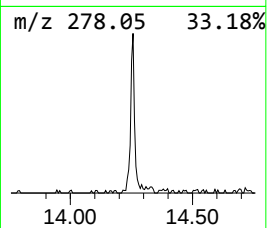
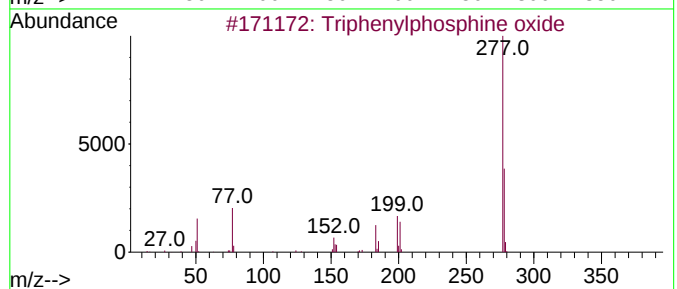
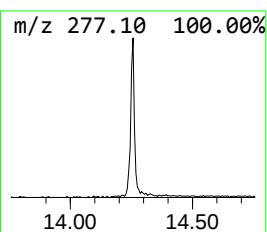
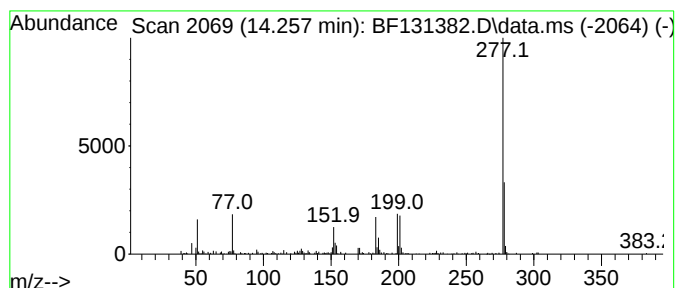
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.257	4.87 ng	147549	Chrysene-d12	14.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
3			(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19N03S	1000483-83-4	58
4			2-Phenyl-6-(trifluoromethyl)-1H...	277	C15H10F3NO	1000387-59-3	42
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	42



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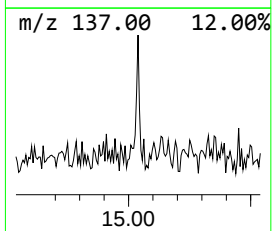
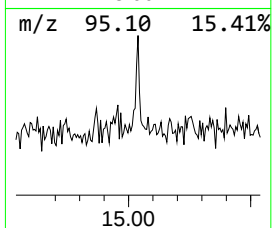
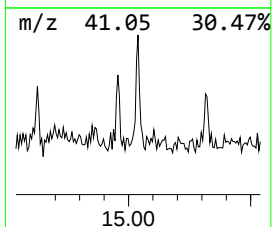
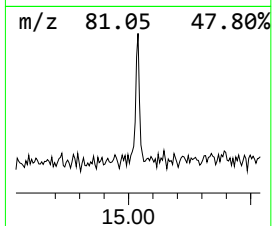
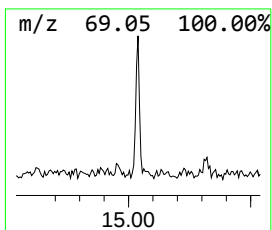
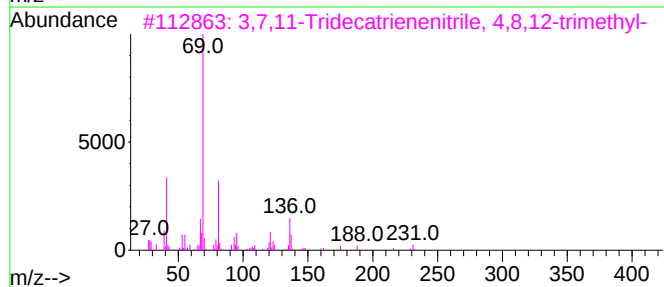
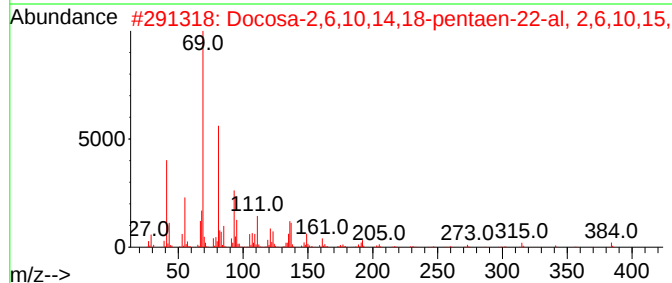
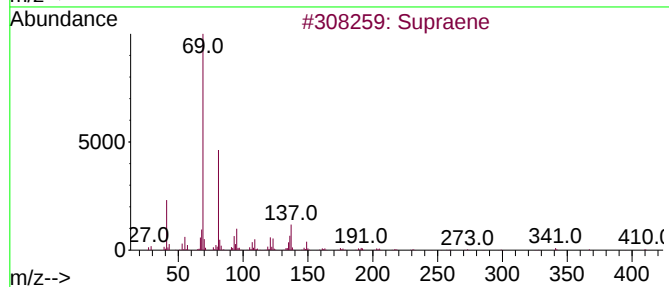
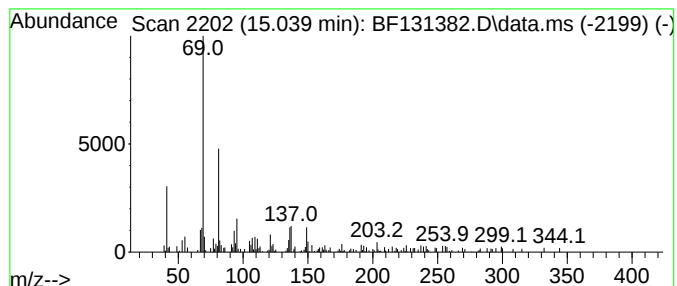
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.039	2.69 ng	60839	Perylene-d12	15.698

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	80
2			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	72
3			3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	64
4			3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	64
5			Furan, 3-(4,8-dimethyl-3,7-nonad...	218	C15H22O	023262-34-2	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112322\
Data File : BF131382.D
Acq On : 24 Nov 2022 02:28
Operator : CG\JU
Sample : N5642-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RIGHT-SIDE-FLATS-26

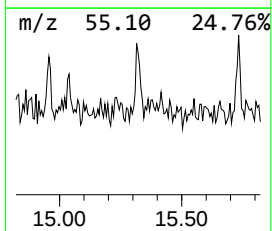
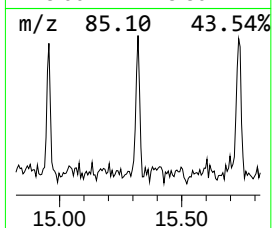
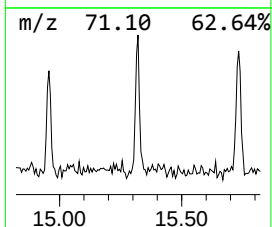
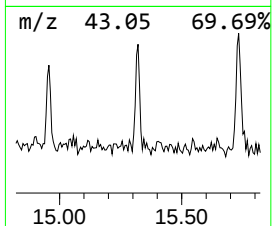
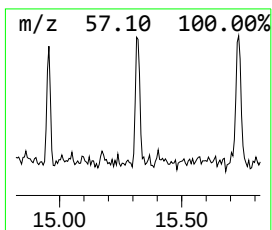
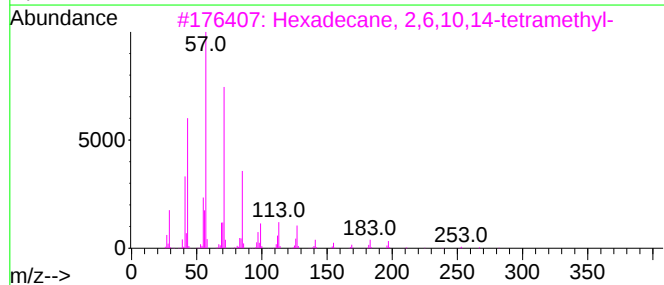
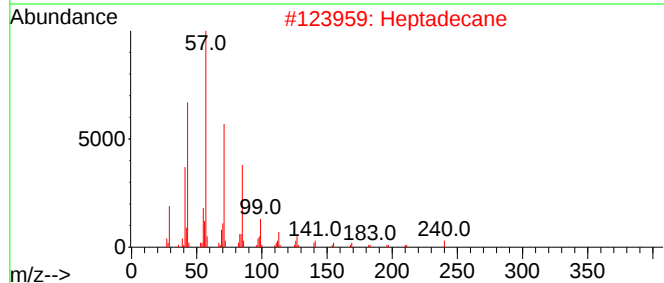
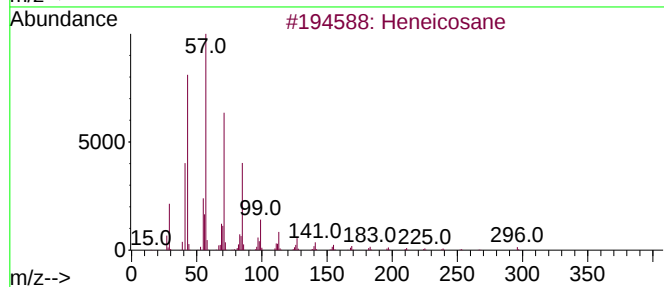
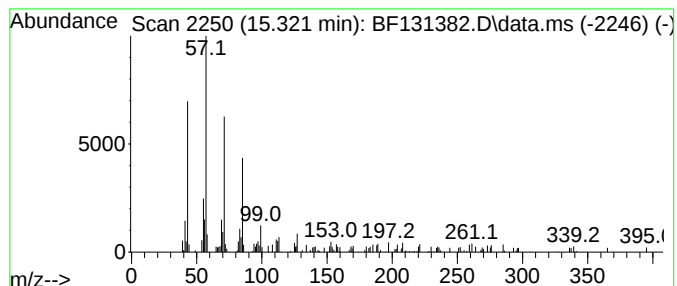
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.321	2.25 ng	50875	Perylene-d12	15.698

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	96
2			Heptadecane	240	C17H36	000629-78-7	91
3			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	90
4			Nonadecane	268	C19H40	000629-92-5	89
5			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112322\
Data File : BF131382.D
Acq On : 24 Nov 2022 02:28
Operator : CG\JU
Sample : N5642-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RIGHT-SIDE-FLATS-26

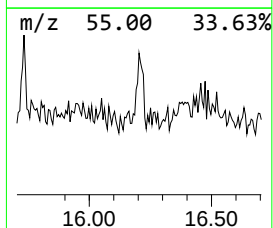
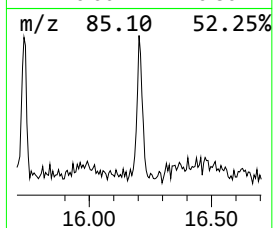
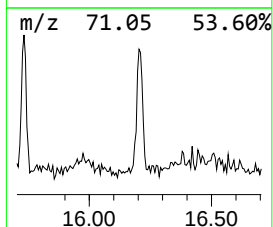
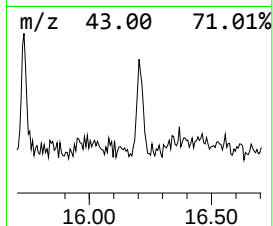
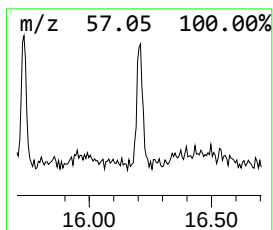
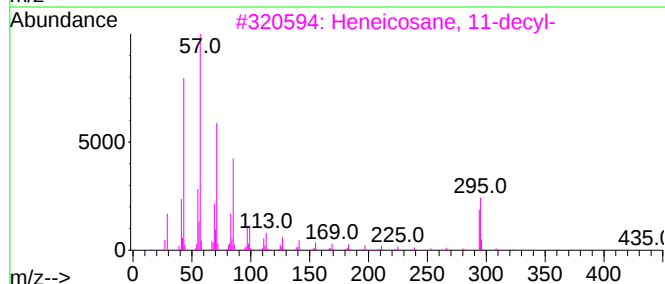
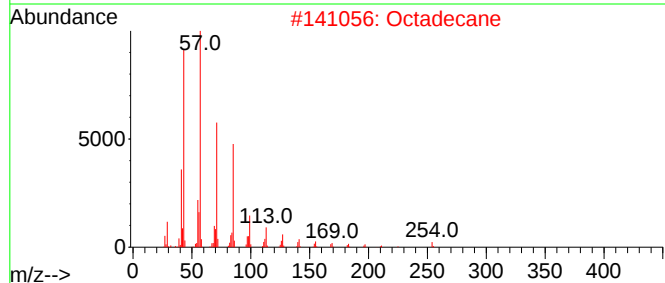
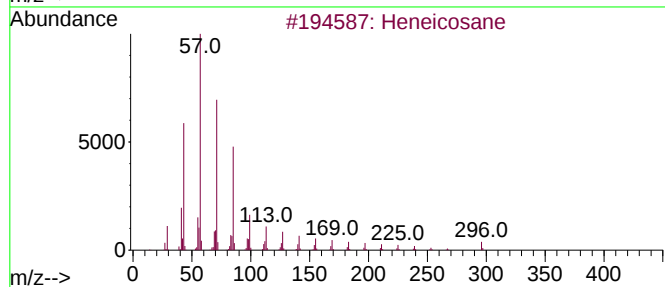
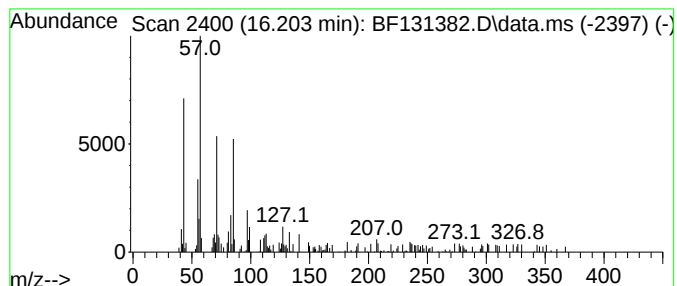
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.203	2.87 ng	64755	Perylene-d12	15.698

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	64
2			Octadecane	254	C18H38	000593-45-3	60
3			Heneicosane, 11-decyl-	437	C31H64	055320-06-4	50
4			Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	49
5			Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112322\
Data File : BF131382.D
Acq On : 24 Nov 2022 02:28
Operator : CG\JU
Sample : N5642-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RIGHT-SIDE-FLATS-26

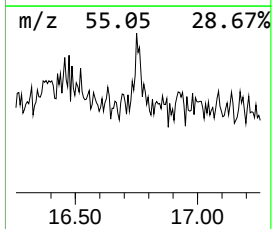
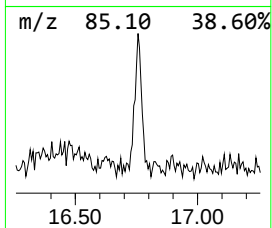
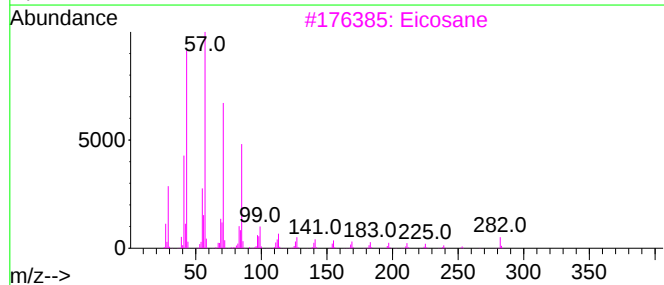
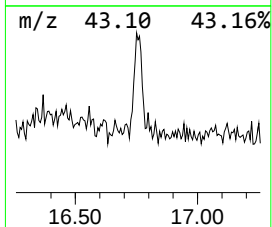
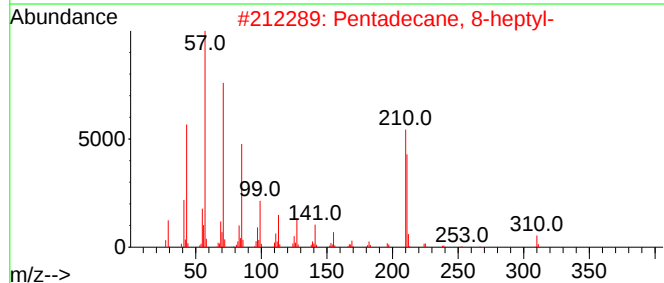
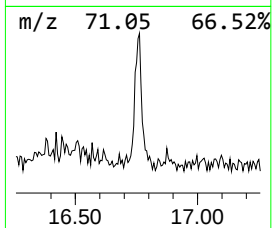
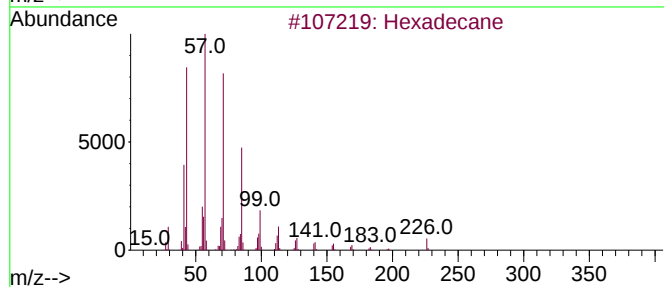
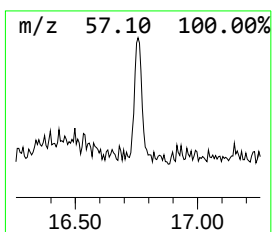
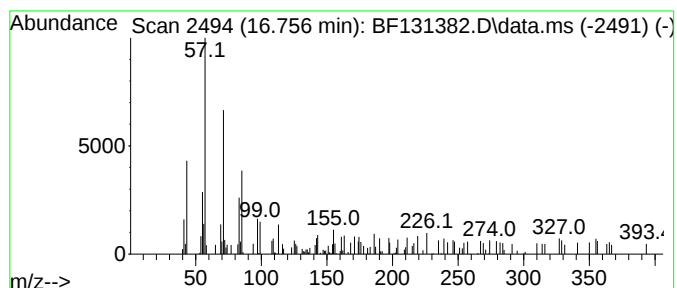
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.756	2.05 ng	46316	Perylene-d12	15.698

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	60
2			Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	53
3			Eicosane	282	C20H42	000112-95-8	53
4			1-Chloroeicosane	316	C20H41Cl	042217-02-7	53
5			Docosane	310	C22H46	000629-97-0	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112322\
Data File : BF131382.D
Acq On : 24 Nov 2022 02:28
Operator : CG\JU
Sample : N5642-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RIGHT-SIDE-FLATS-26

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...	2.299	32.4	ng	1144290	1	6.957	706024	20.0
2-Pentanone, 4-...	5.187	11.0	ng	389713	1	6.957	706024	20.0
n-Hexadecanoic ...	12.021	4.0	ng	135174	4	11.504	668733	20.0
3-Octadecene, (E)-	14.033	12.5	ng	377968	5	14.157	606467	20.0
Triphenylphosph...	14.257	4.9	ng	147549	5	14.157	606467	20.0
Supraene	15.039	2.7	ng	60839	6	15.698	451622	20.0
Heneicosane	15.321	2.3	ng	50875	6	15.698	451622	20.0
Octadecane	16.203	2.9	ng	64755	6	15.698	451622	20.0
Hexadecane	16.756	2.0	ng	46316	6	15.698	451622	20.0