

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF052419\
 Data File : BF114586.D
 Acq On : 24 May 2019 22:44
 Operator : JU/SJ
 Sample : K3026-16
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-3-S

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-BF051019.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.746	107	112	128	rVB	210622	349468	7.51%	0.998%
2	4.610	425	429	440	rBV	108660	152447	3.28%	0.435%
3	5.040	499	502	517	rVB2	266967	462006	9.93%	1.319%
4	5.457	569	573	599	rBV	2760343	3386306	72.75%	9.668%
5	6.463	740	744	762	rBV	2743722	3184960	68.42%	9.093%
6	6.593	762	766	781	rVB	4082344	3757255	80.72%	10.727%
7	6.810	800	803	813	rBV	857806	763247	16.40%	2.179%
8	6.969	826	830	842	rBV	3300837	2853165	61.30%	8.146%
9	7.375	895	899	915	rBV	2513449	2487795	53.45%	7.103%
10	8.092	1017	1021	1039	rBV	1013332	964514	20.72%	2.754%
11	9.169	1200	1204	1207	rBV	4708478	4143331	89.01%	11.829%
12	9.845	1316	1319	1330	rVB2	1147287	1057410	22.72%	3.019%
13	10.639	1450	1454	1474	rBV	2581733	2812250	60.42%	8.029%
14	11.333	1569	1572	1580	rBV	1341109	1165148	25.03%	3.327%
15	12.916	1837	1841	1845	rBV	4659469	4654740	100.00%	13.290%
16	13.980	2018	2022	2031	rBV	1041203	1037994	22.30%	2.964%
17	14.427	2094	2098	2104	rBV	84224	85047	1.83%	0.243%
18	14.727	2145	2149	2153	rBV	134322	132346	2.84%	0.378%
19	15.057	2201	2205	2210	rVB	143598	161686	3.47%	0.462%
20	15.439	2263	2270	2280	rBV	683615	1077031	23.14%	3.075%
21	15.851	2334	2340	2347	rBV	120658	195489	4.20%	0.558%
22	16.339	2418	2423	2429	rVB	82076	141923	3.05%	0.405%

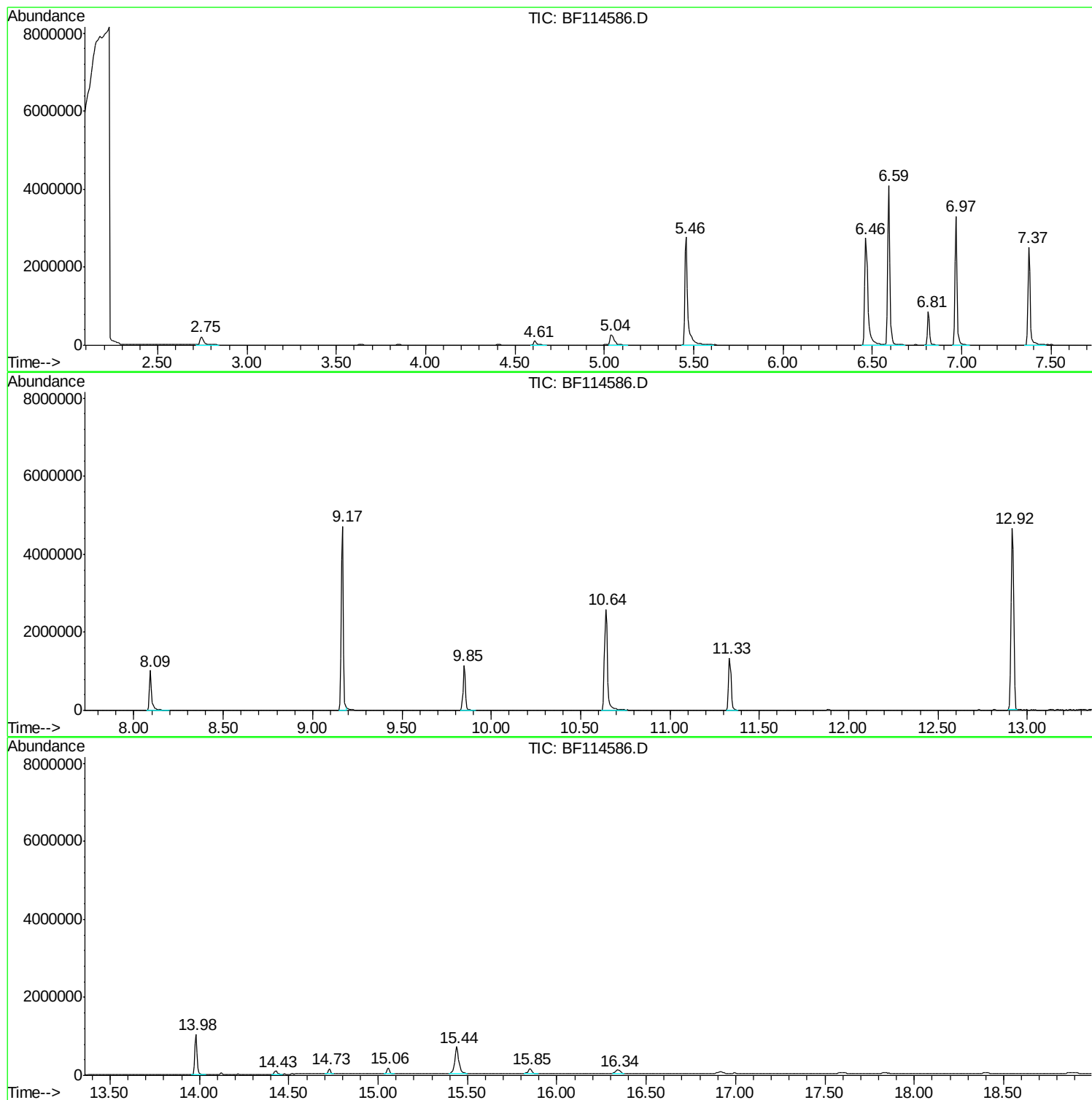
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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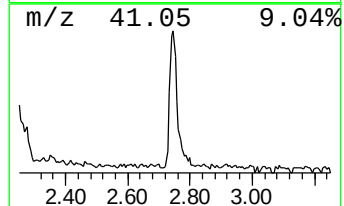
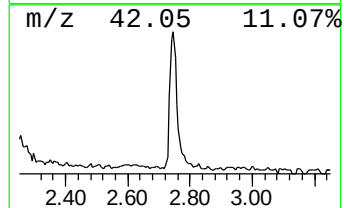
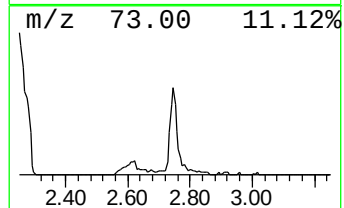
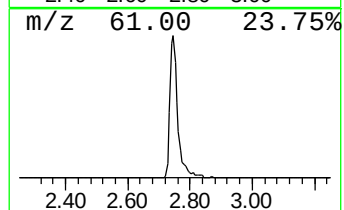
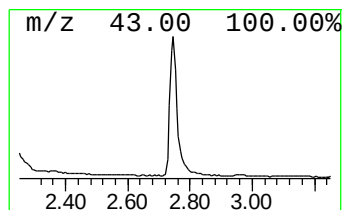
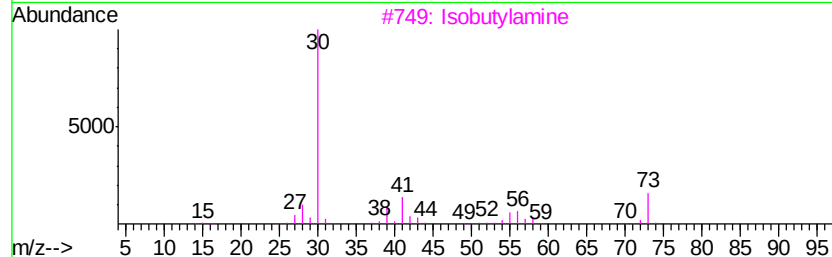
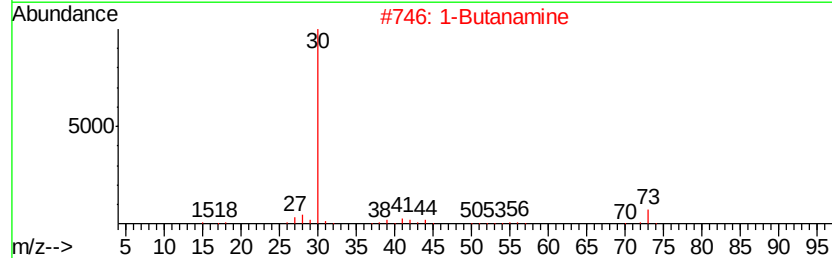
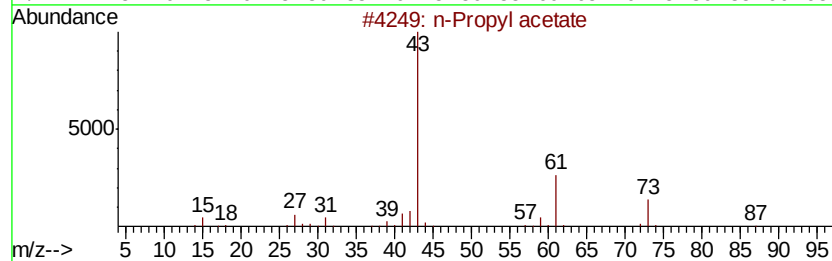
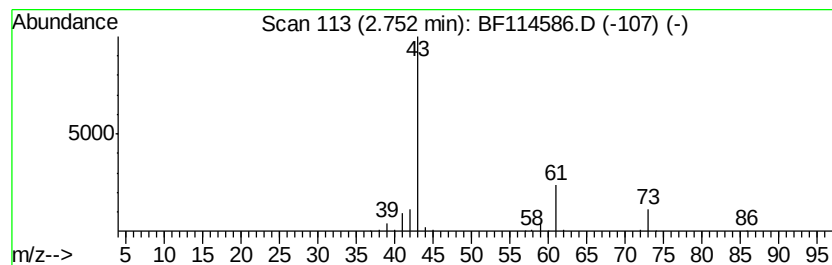
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.75	9.16 ng	349468	1,4-Dichlorobenzene-d4	6.81	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	1-Butanamine	73	C4H11N	000109-73-9	7
3	Isobutylamine	73	C4H11N	000078-81-9	7
4	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	4
5	Hydrogen azide	43	HN3	007782-79-8	4



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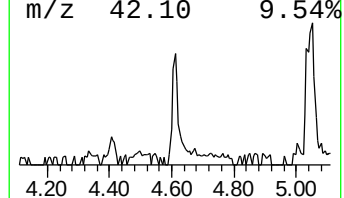
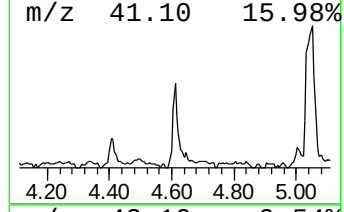
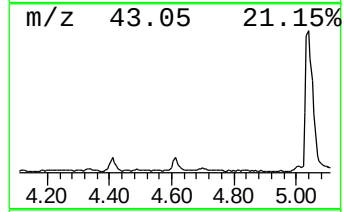
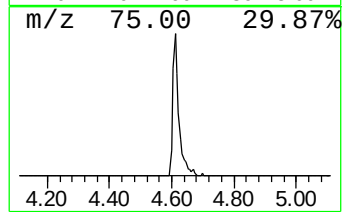
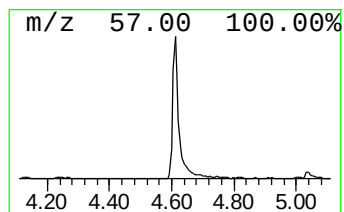
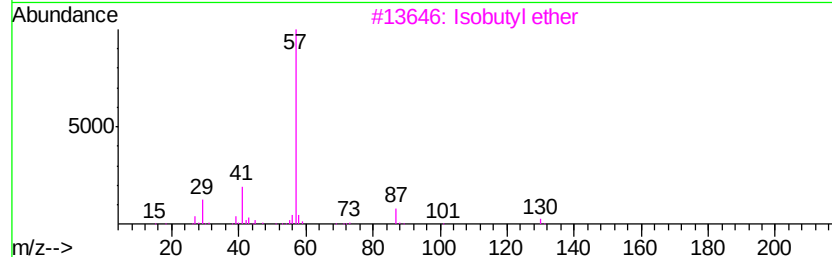
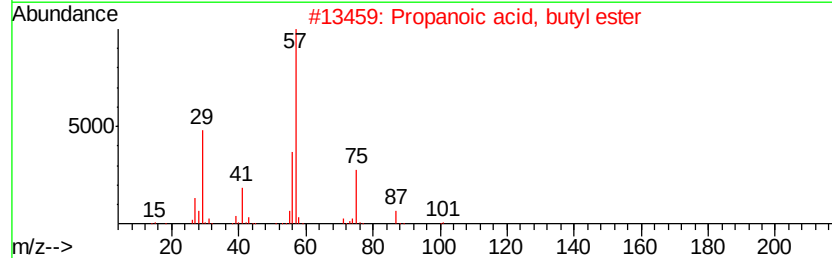
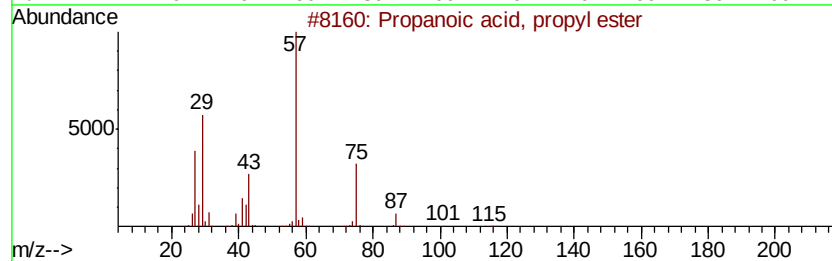
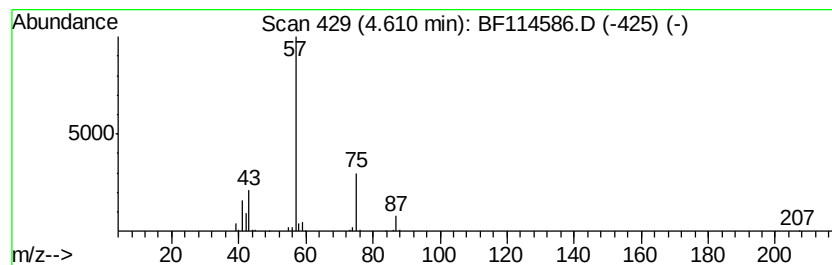
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Peak Number 2 Propanoic acid, propyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.61	3.99 ng	152447	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
2		Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	36
3		Isobutyl ether	130	C8H18O	000628-55-7	23
4		di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	16
5		3-Pentanol, 3-(1,1-dimethylethyl...	200	C13H28O	041902-42-5	16



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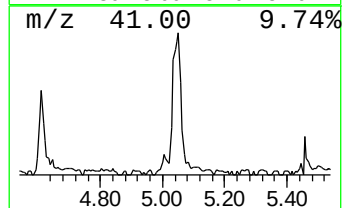
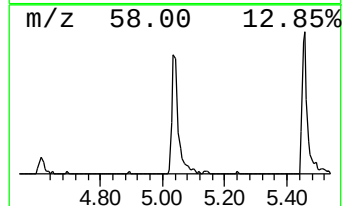
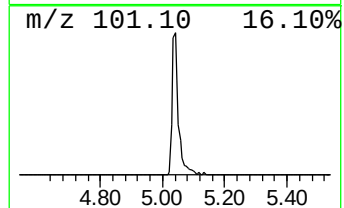
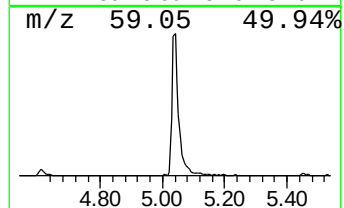
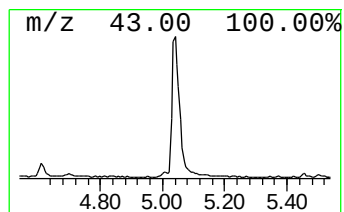
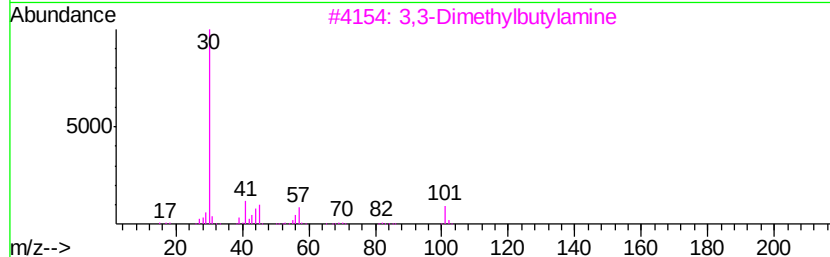
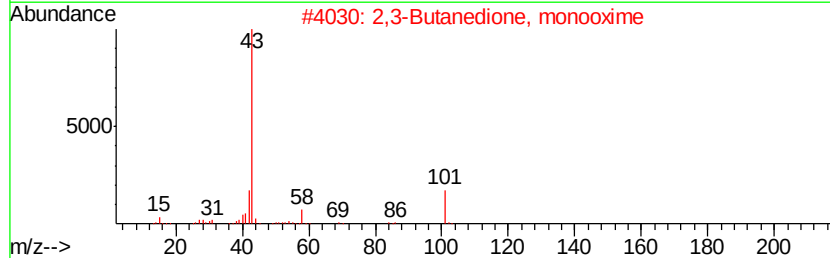
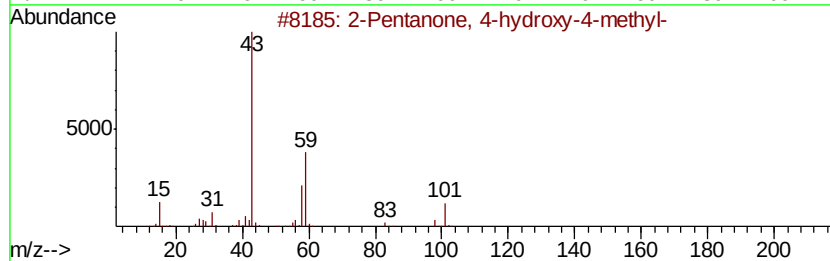
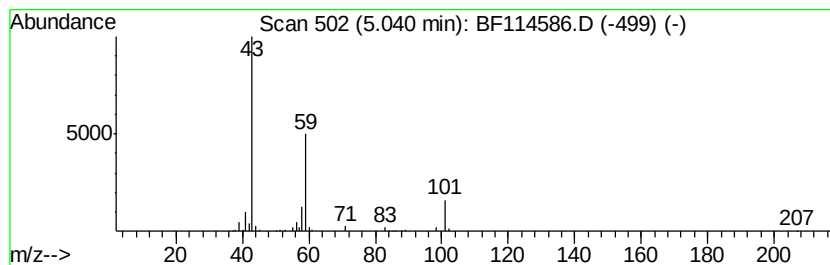
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	12.11 ng	462006	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3		3,3-Dimethylbutylamine	101	C6H15N	015673-00-4	9
4		Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9
5		Dimethadione	129	C5H7NO3	000695-53-4	9



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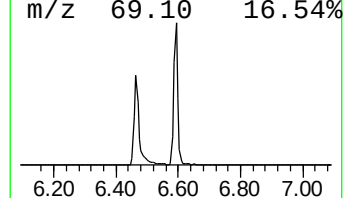
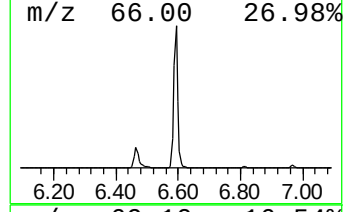
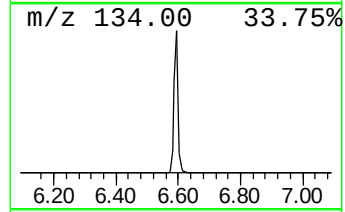
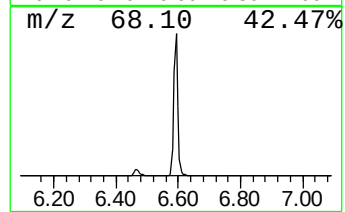
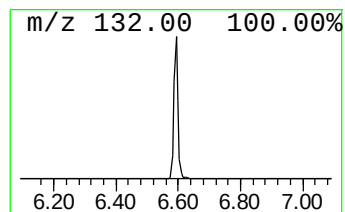
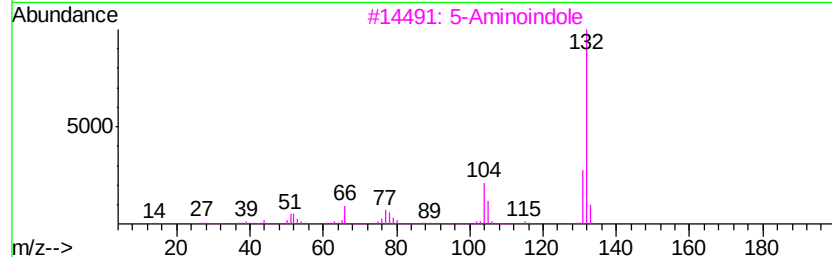
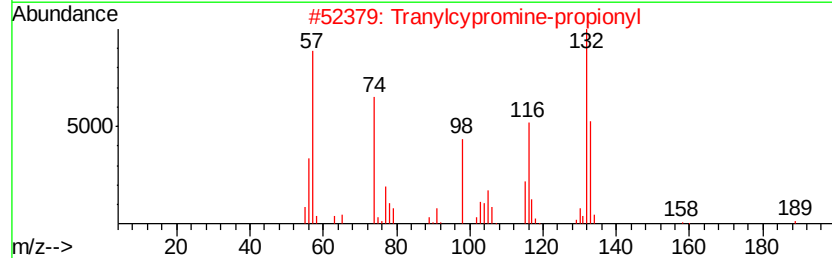
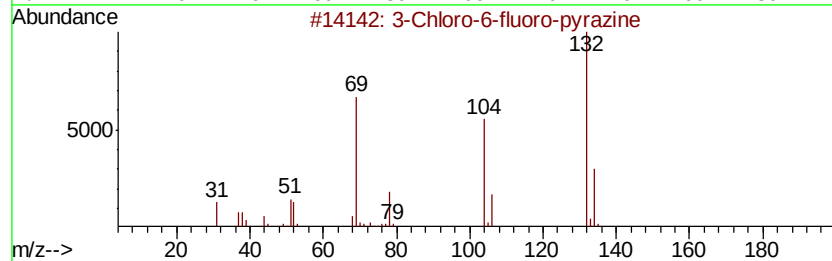
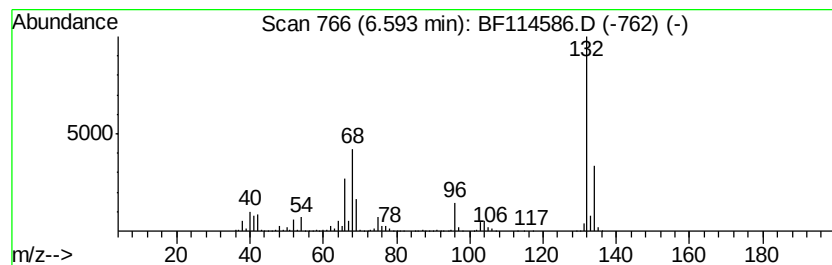
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Peak Number 4 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	98.45 ng	3757260	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3			5-Aminoindole	132	C8H8N2	005192-03-0	12
4			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
5			1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9



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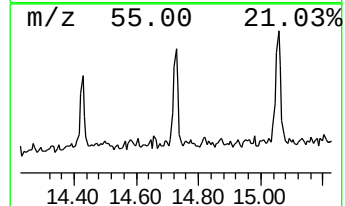
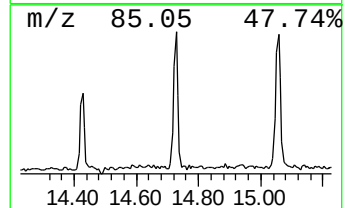
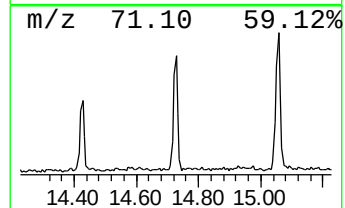
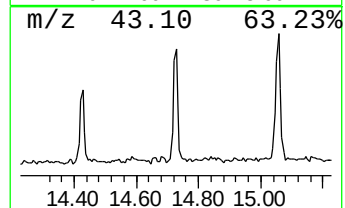
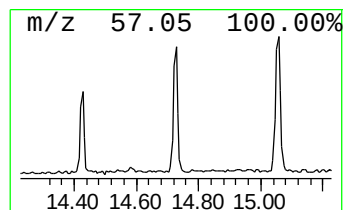
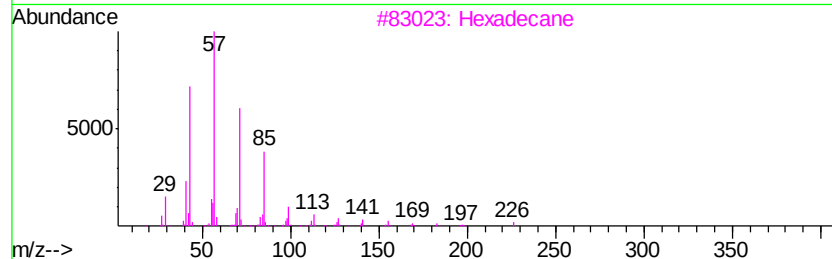
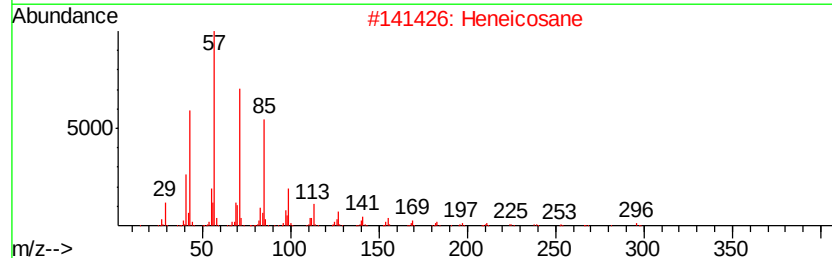
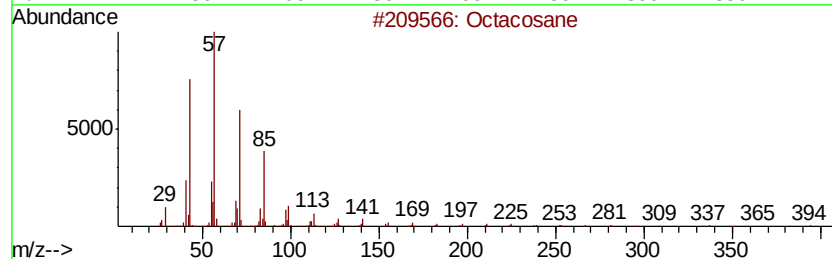
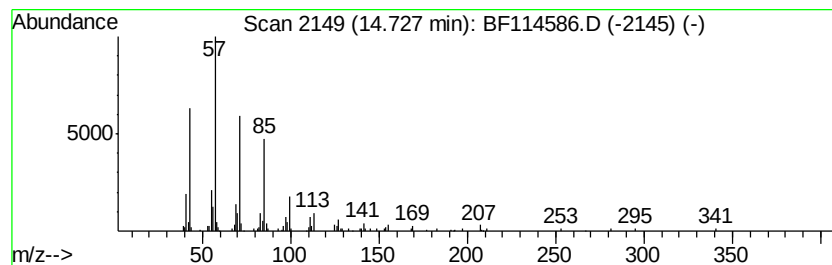
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Peak Number 6 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	2.46 ng	132346	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Hexadecane	226	C16H34	000544-76-3	91
4		Octadecane	254	C18H38	000593-45-3	91
5		Eicosane	282	C20H42	000112-95-8	91



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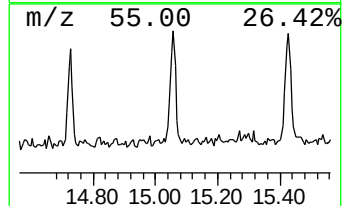
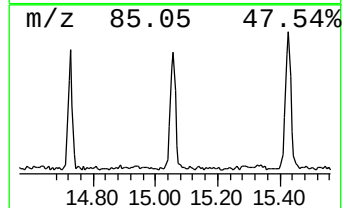
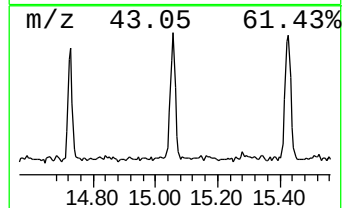
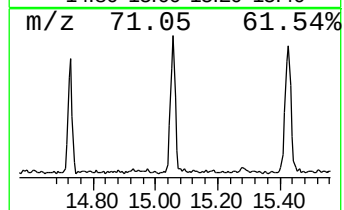
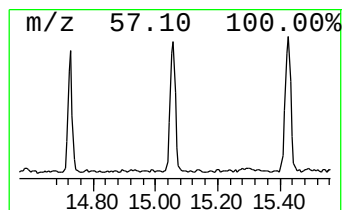
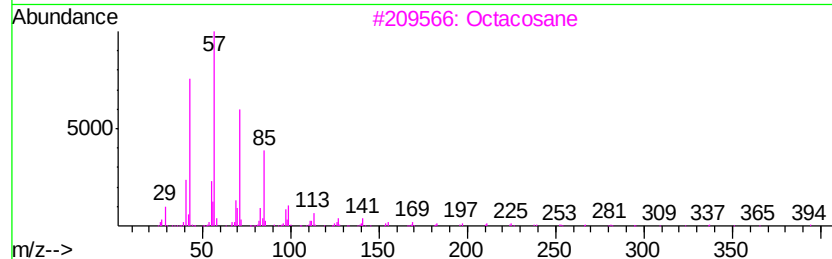
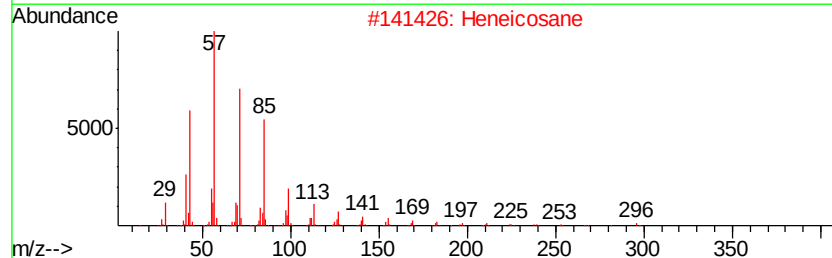
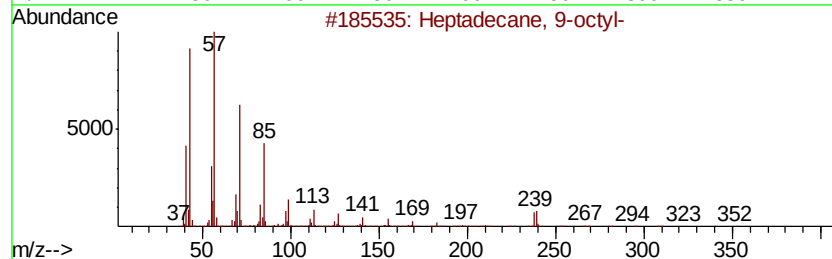
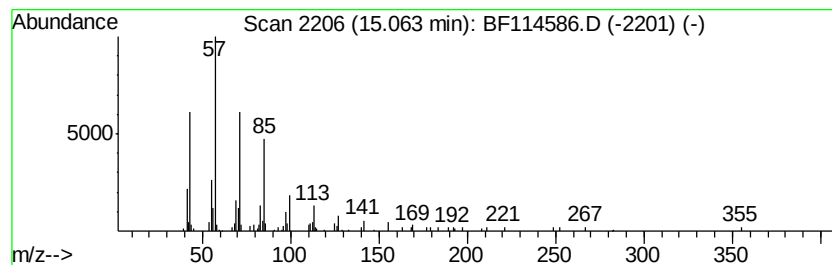
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF051019.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 7 Heptadecane, 9-octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	3.00 ng	161686	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Hentriacontane	437	C31H64	000630-04-6	91
5		Heptacosane	380	C27H56	000593-49-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052419\
Data File : BF114586.D
Acq On : 24 May 2019 22:44
Operator : JU/SJ
Sample : K3026-16
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3-S

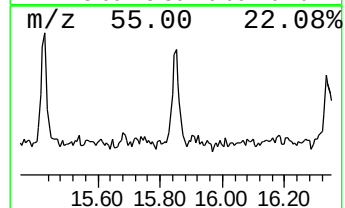
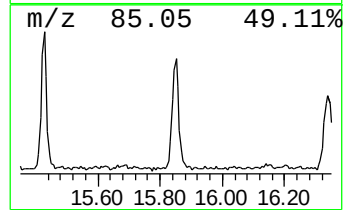
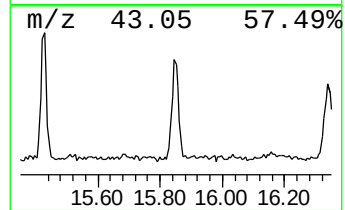
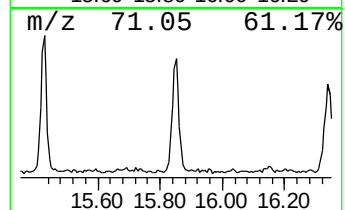
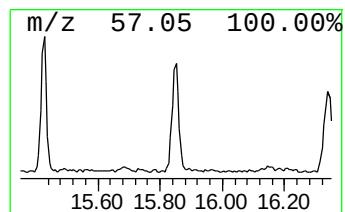
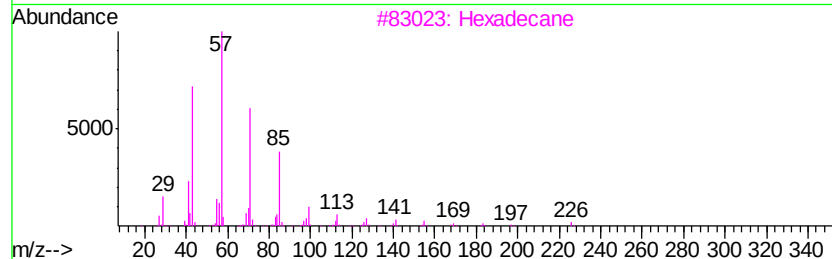
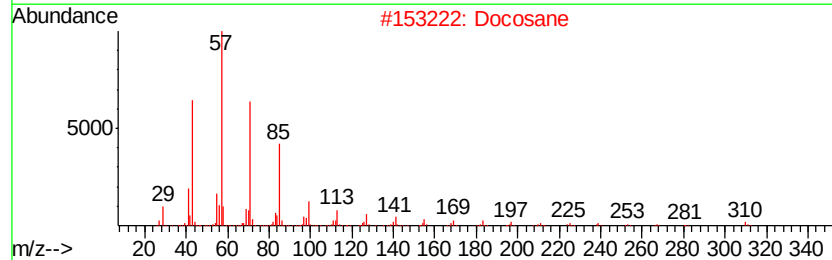
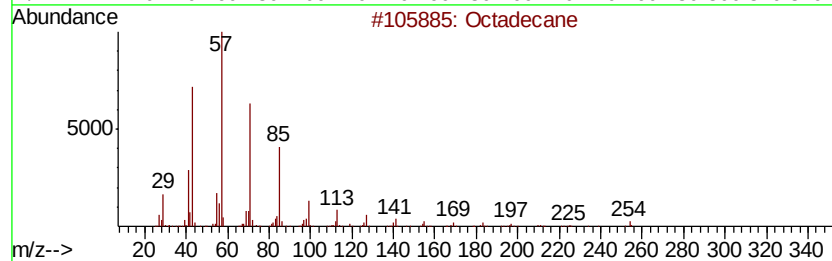
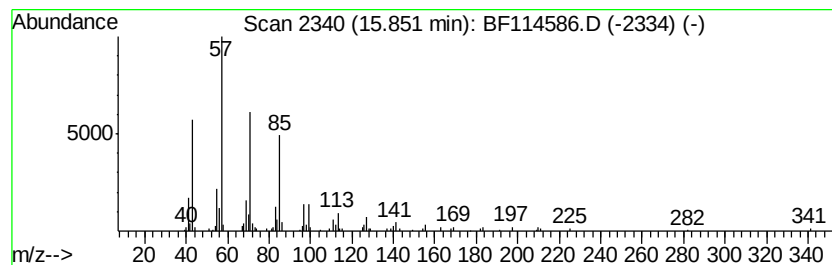
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.85	3.63 ng	195489	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	87
2		Docosane	310	C22H46	000629-97-0	87
3		Hexadecane	226	C16H34	000544-76-3	86
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
5		Tetracosane	338	C24H50	000646-31-1	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052419\
Data File : BF114586.D
Acq On : 24 May 2019 22:44
Operator : JU/SJ
Sample : K3026-16
Misc :
ALS Vial : 15 Sample Multiplier: 1

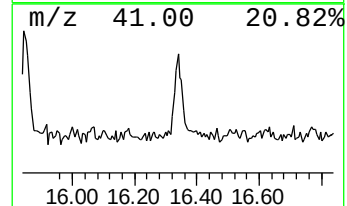
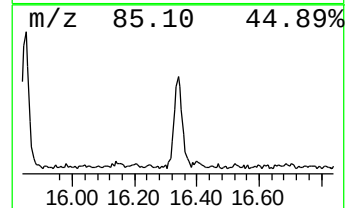
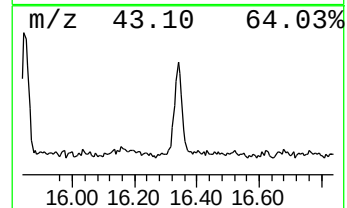
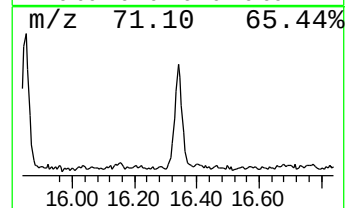
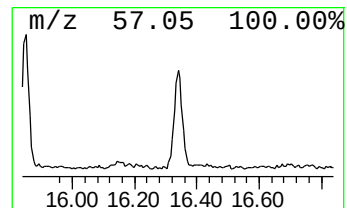
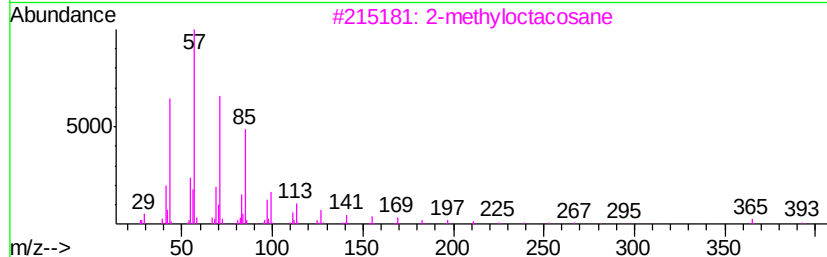
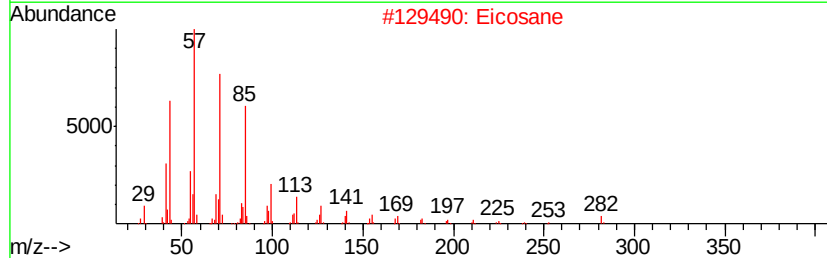
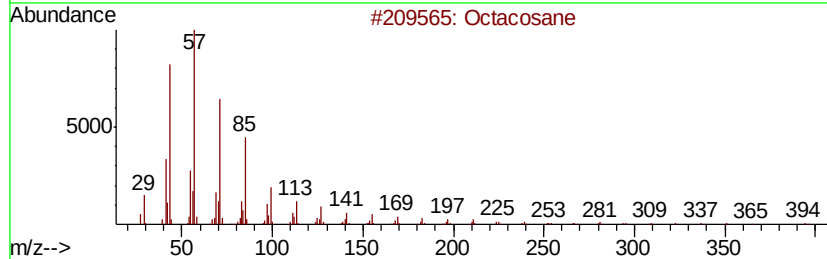
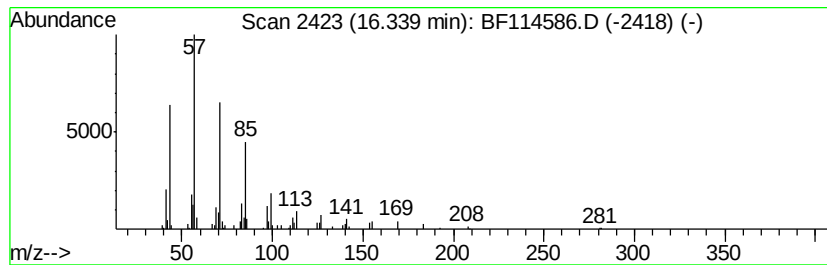
Instrument :
BNA_F
ClientSampleId :
TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
16.34	2.64 ng	141923	Perylene-d12		15.44
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Eicosane	282	C20H42	000112-95-8	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Tetratetracontane	619	C44H90	007098-22-8	91
5	Hentriacontane	437	C31H64	000630-04-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF052419\
Data File : BF114586.D
Acq On : 24 May 2019 22:44
Operator : JU/SJ
Sample : K3026-16
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	2.75	9.2	ng	349468	1	6.81	763247	20.0
Propanoic acid, p...	4.61	4.0	ng	152447	1	6.81	763247	20.0
2-Pentanone, 4-hy...	5.04	12.1	ng	462006	1	6.81	763247	20.0
unknown6.59	6.59	98.5	ng	3757260	1	6.81	763247	20.0
Octacosane	14.73	2.5	ng	132346	6	15.44	1077030	20.0
Heptadecane, 9-oc...	15.06	3.0	ng	161686	6	15.44	1077030	20.0
Octadecane	15.85	3.6	ng	195489	6	15.44	1077030	20.0
Eicosane	16.34	2.6	ng	141923	6	15.44	1077030	20.0