

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF052219\
 Data File : BF114485.D
 Acq On : 22 May 2019 14:58
 Operator : JU/SJ
 Sample : PB119674BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB119674BL

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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	2.163	10	13	19	rVB	131149	183663	3.36%	0.434%
2	5.057	501	505	516	rBV	299104	419621	7.68%	0.992%
3	5.469	571	575	595	rBV	2914870	3287007	60.18%	7.768%
4	6.469	741	745	764	rBV	2855293	3367554	61.65%	7.958%
5	6.604	764	768	783	rVB	3722692	3318824	60.76%	7.843%
6	6.828	802	806	817	rVB	1439770	1240291	22.71%	2.931%
7	6.987	828	833	851	rBV	3859888	3746856	68.60%	8.855%
8	7.392	897	902	922	rBV	2914306	3167441	57.99%	7.485%
9	8.110	1019	1024	1045	rBV	1467121	1602463	29.34%	3.787%
10	9.186	1201	1207	1222	rBV	5301241	5462186	100.00%	12.908%
11	9.869	1318	1323	1341	rBV	1551883	1788910	32.75%	4.228%
12	10.657	1453	1457	1484	rBV	1996153	2392667	43.80%	5.654%
13	11.351	1572	1575	1591	rBV	1729157	1966794	36.01%	4.648%
14	12.933	1840	1844	1848	rBV	5085863	5235840	95.86%	12.373%
15	13.998	2021	2025	2035	rBV	1788064	1873993	34.31%	4.429%
16	14.451	2097	2102	2107	rBV	134129	134443	2.46%	0.318%
17	14.757	2149	2154	2159	rVB	245338	256070	4.69%	0.605%
18	15.086	2204	2210	2218	rBV	268810	346401	6.34%	0.819%
19	15.474	2269	2276	2295	rBV	1284792	2189261	40.08%	5.174%
20	15.892	2341	2347	2353	rVB	140960	216356	3.96%	0.511%
21	16.386	2425	2431	2440	rVB2	64276	118843	2.18%	0.281%

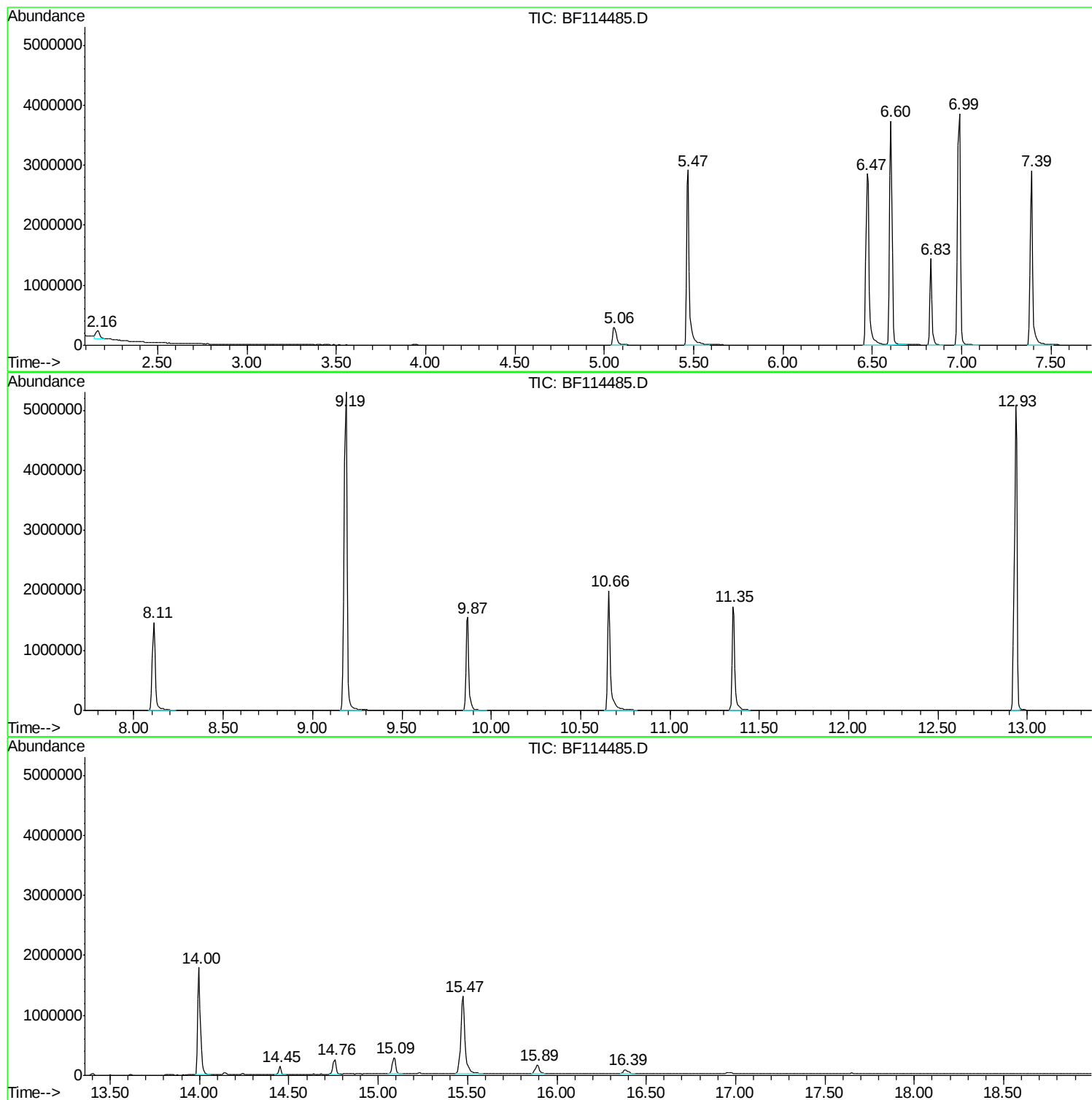
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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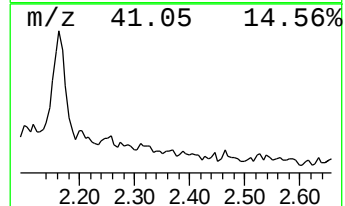
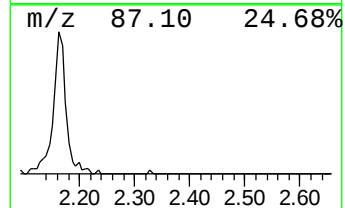
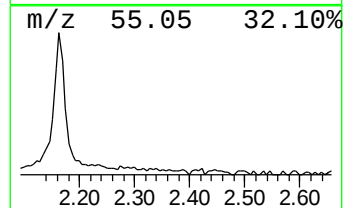
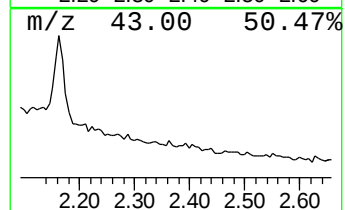
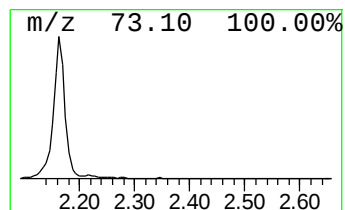
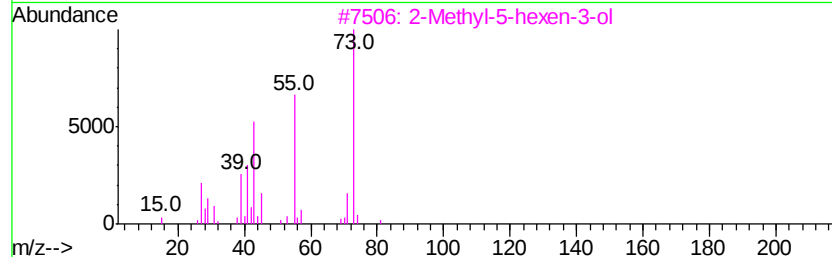
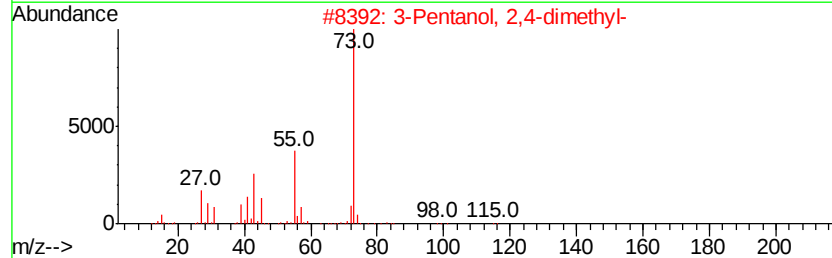
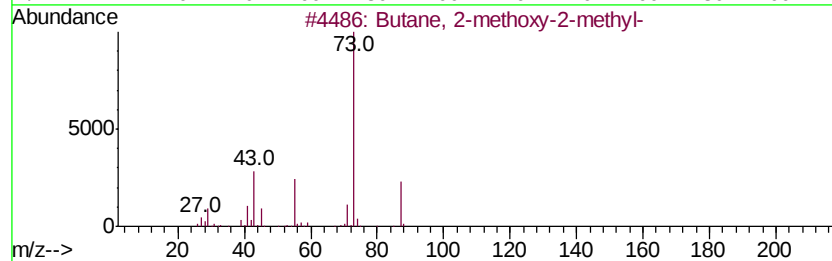
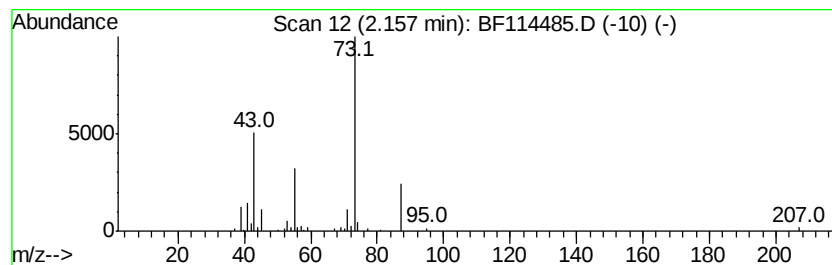
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	2.96 ng	183663	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
3		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28
4		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	25
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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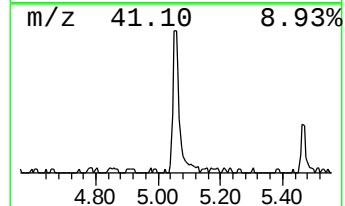
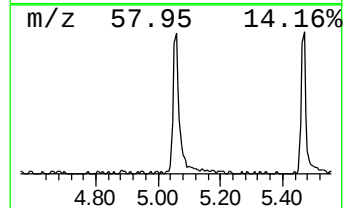
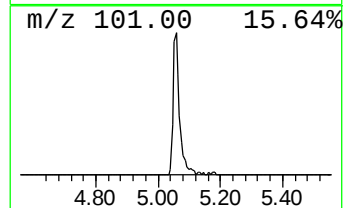
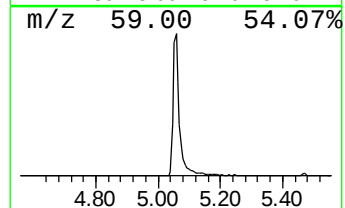
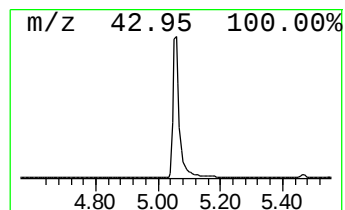
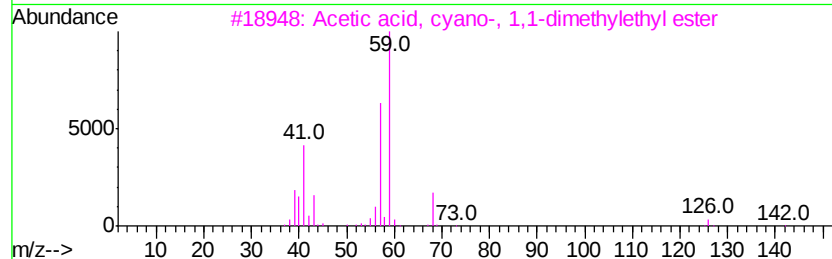
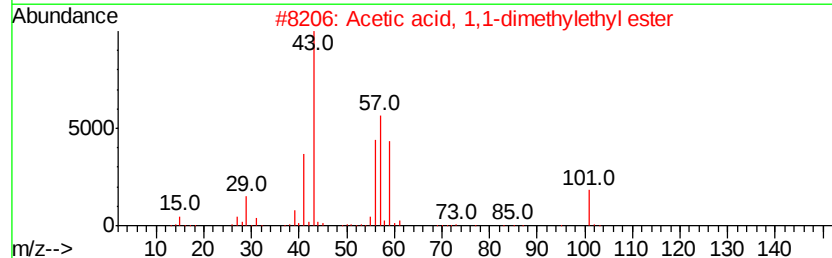
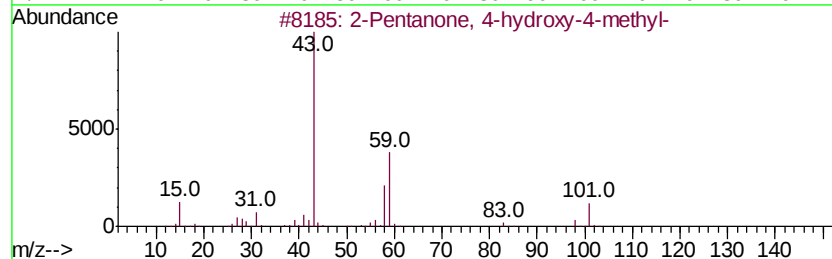
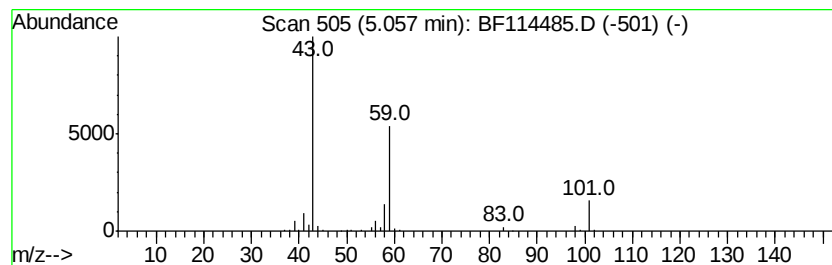
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
5.06	6.77 ng	419621	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
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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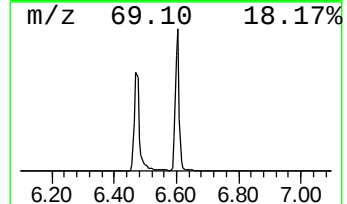
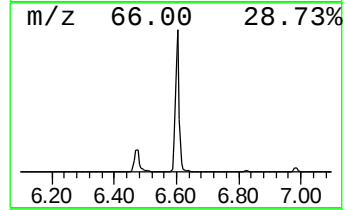
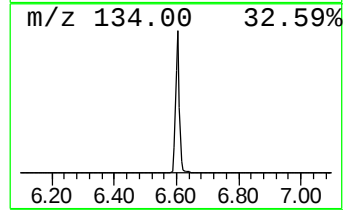
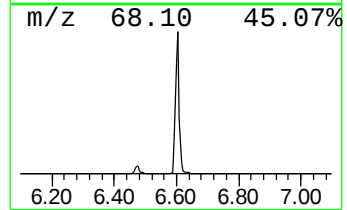
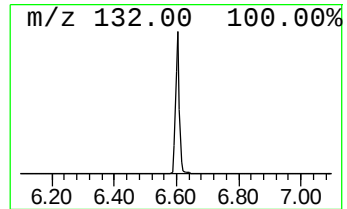
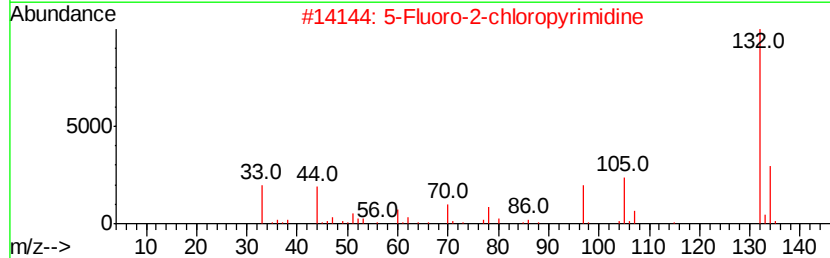
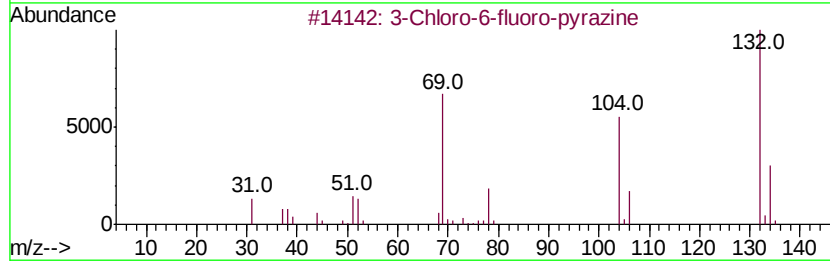
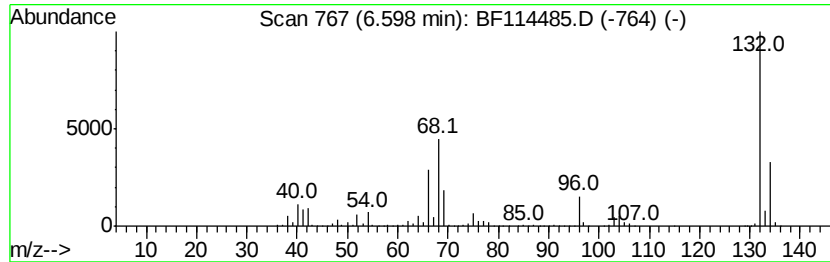
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Peak Number 3 unknown6.60 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.
6.60	53.52 ng	3318820	1,4-Dichlorobenzene-d4		6.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole			132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl			189	C12H15NO	1000123-86-3	10
5	Imidazole, 4,5-dicyano-1-methyl-			132	C6H4N4	019485-35-9	9



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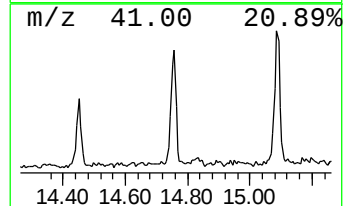
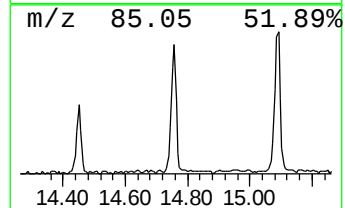
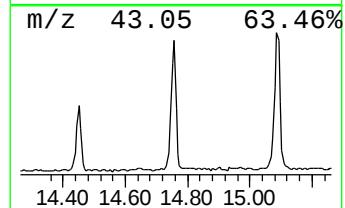
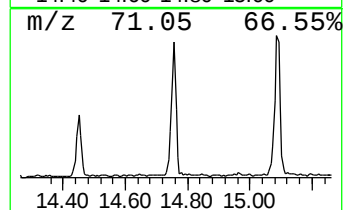
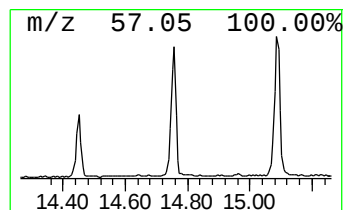
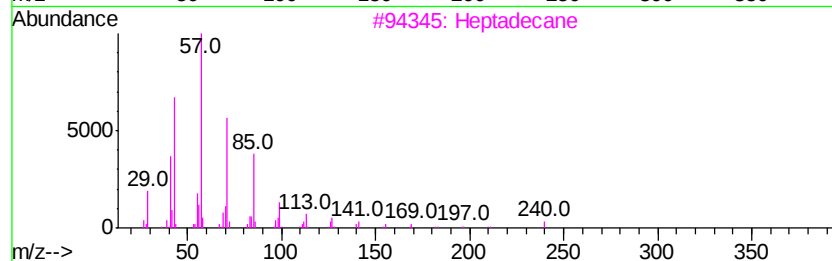
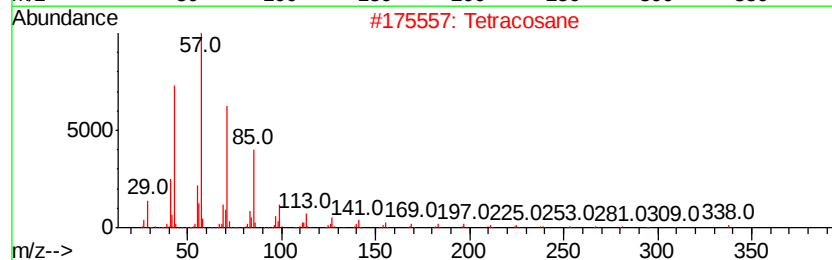
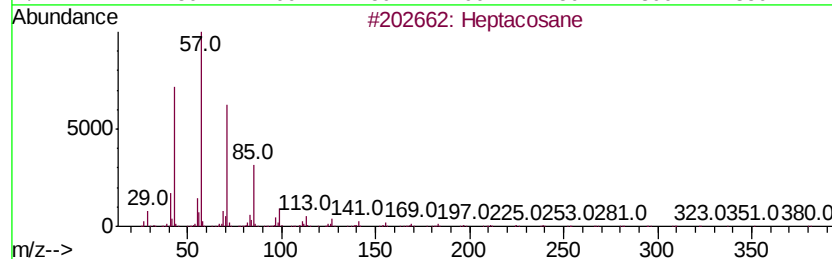
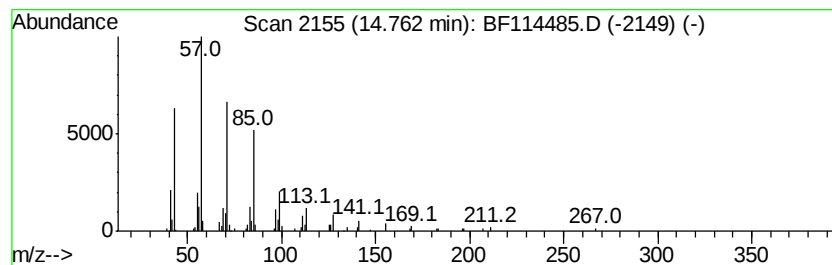
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.76	2.34 ng	256070	Perylene-d12	15.47

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Tetracosane		338	C24H50	000646-31-1	91
3	Heptadecane		240	C17H36	000629-78-7	91
4	Octacosane		394	C28H58	000630-02-4	91
5	Heneicosane		296	C21H44	000629-94-7	90



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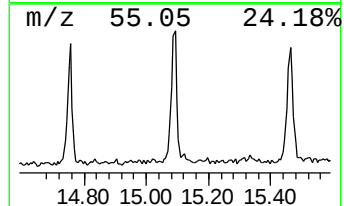
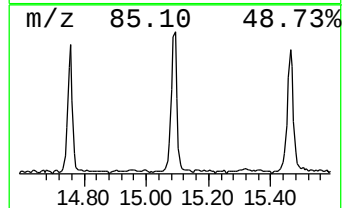
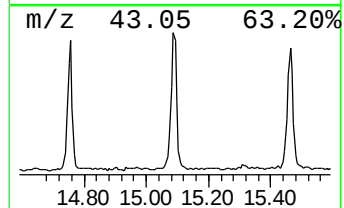
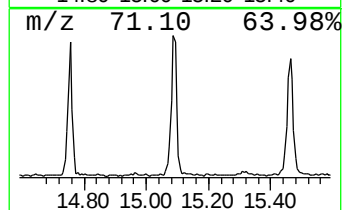
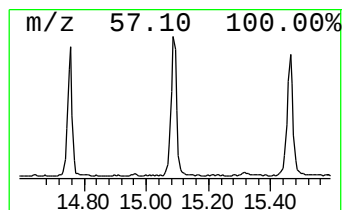
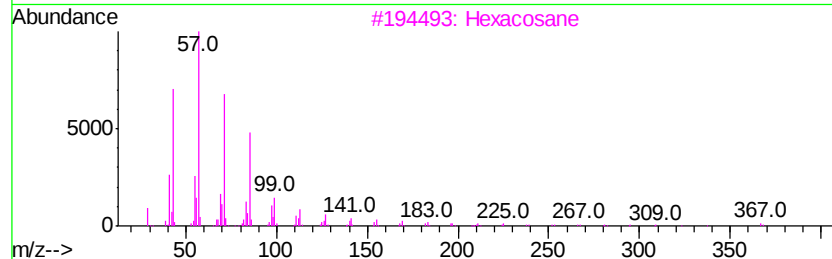
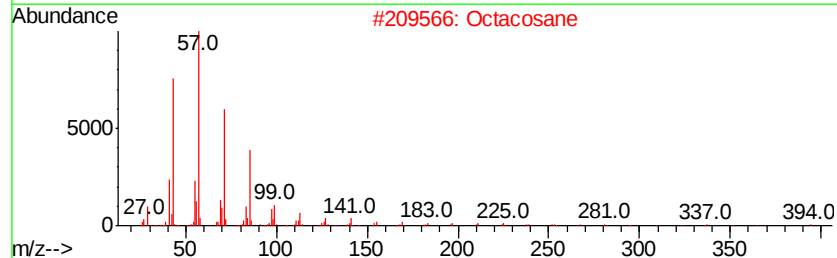
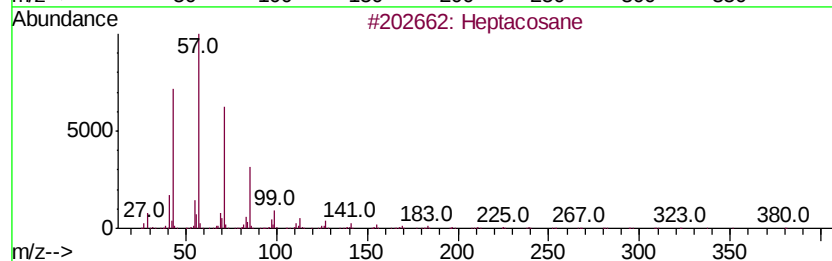
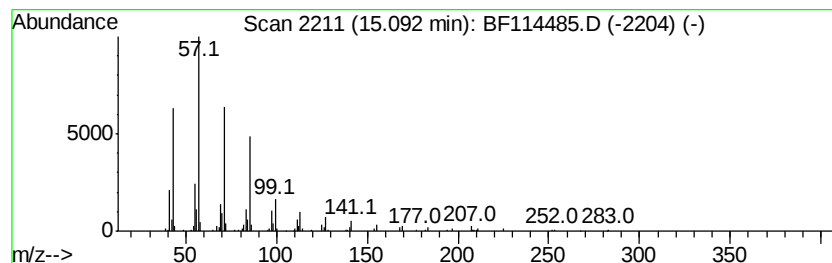
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	3.16 ng	346401	Perylene-d12	15.47

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Octacosane		394	C28H58	000630-02-4	91
3	Hexacosane		366	C26H54	000630-01-3	91
4	Heptadecane		240	C17H36	000629-78-7	91
5	Heneicosane		296	C21H44	000629-94-7	90



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.16	3.0	ng	183663	1	6.83	1240290	20.0
2-Pentanone, 4-hy...	5.06	6.8	ng	419621	1	6.83	1240290	20.0
unknown6.60	6.60	53.5	ng	3318820	1	6.83	1240290	20.0
Heptacosane	14.76	2.3	ng	256070	6	15.47	2189260	20.0
Octacosane	15.09	3.2	ng	346401	6	15.47	2189260	20.0