

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052620\
 Data File : BG045469.D
 Acq On : 26 May 2020 22:59
 Operator : CG/JU
 Sample : L2744-13
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 NM42-COMP-2020-0-6

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_G\METHODS\8270-BG051520.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	3.114	3	4	16	rVB	139673	190249	4.44%	0.647%
2	5.563	413	421	432	rBV	870544	1479710	34.53%	5.030%
3	7.179	688	696	707	rBV	980492	1745636	40.74%	5.934%
4	7.960	822	829	837	rBV	307177	542749	12.67%	1.845%
5	8.289	876	885	895	rBV	874473	1597616	37.28%	5.430%
6	9.123	1017	1027	1040	rBV	674727	1268262	29.60%	4.311%
7	10.768	1299	1307	1319	rBV	422415	775775	18.10%	2.637%
8	13.229	1718	1726	1740	rBV	1882426	3140644	73.29%	10.675%
9	14.052	1859	1866	1876	rBV	198004	313862	7.32%	1.067%
10	14.604	1953	1960	1968	rBV2	668276	1080507	25.21%	3.673%
11	16.102	2208	2215	2231	rBV	1471977	2380572	55.55%	8.092%
12	17.353	2419	2428	2432	rBV	800574	1278321	29.83%	4.345%
13	17.394	2432	2435	2440	rVB	169677	242508	5.66%	0.824%
14	18.276	2583	2585	2589	rVB2	31417	43851	1.02%	0.149%
15	18.422	2604	2610	2614	rBV2	39338	72491	1.69%	0.246%
16	19.403	2772	2777	2783	rVB	322436	462667	10.80%	1.573%
17	19.762	2829	2838	2847	rBV	274671	494992	11.55%	1.683%
18	19.967	2866	2873	2880	rBV	3281389	4285295	100.00%	14.566%
19	20.020	2880	2882	2887	rVB6	31728	45120	1.05%	0.153%
20	20.361	2936	2940	2945	rBV4	31549	60529	1.41%	0.206%
21	20.819	3014	3018	3026	rVB4	60672	110922	2.59%	0.377%
22	20.919	3030	3035	3039	rBV7	50253	94740	2.21%	0.322%
23	21.013	3048	3051	3056	rVB2	33368	51553	1.20%	0.175%
24	21.160	3073	3076	3086	rVB7	78152	125110	2.92%	0.425%
25	21.266	3090	3094	3102	rVB4	177912	310017	7.23%	1.054%
26	21.606	3144	3152	3158	rBV2	821886	1618132	37.76%	5.500%
27	21.653	3158	3160	3174	rVB	146570	266531	6.22%	0.906%
28	21.806	3183	3186	3192	rVB3	62620	91344	2.13%	0.310%
29	21.947	3200	3210	3215	rBV2	466344	1004313	23.44%	3.414%
30	22.194	3247	3252	3258	rBV5	219519	390097	9.10%	1.326%
31	22.411	3284	3289	3301	rVB3	110647	242931	5.67%	0.826%
32	22.740	3341	3345	3352	rVB10	38549	77929	1.82%	0.265%
33	23.087	3400	3404	3412	rVB3	108671	211971	4.95%	0.721%
34	23.422	3458	3461	3472	rVB8	64252	133926	3.13%	0.455%

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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_G\METHODS\8270-BG051520.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	23.762	3512	3519	3526	rBV2	98232	303946	7.09%	1.033%
36	23.874	3533	3538	3544	rVV	131101	258947	6.04%	0.880%
37	23.938	3545	3549	3557	rVB5	63667	136976	3.20%	0.466%
38	24.614	3654	3664	3671	rBV	80335	251694	5.87%	0.856%
39	24.761	3680	3689	3709	rVB3	462542	1635820	38.17%	5.560%
40	25.912	3876	3885	3894	rVB2	158113	452378	10.56%	1.538%
41	27.228	4104	4109	4121	rVB7	42720	149070	3.48%	0.507%

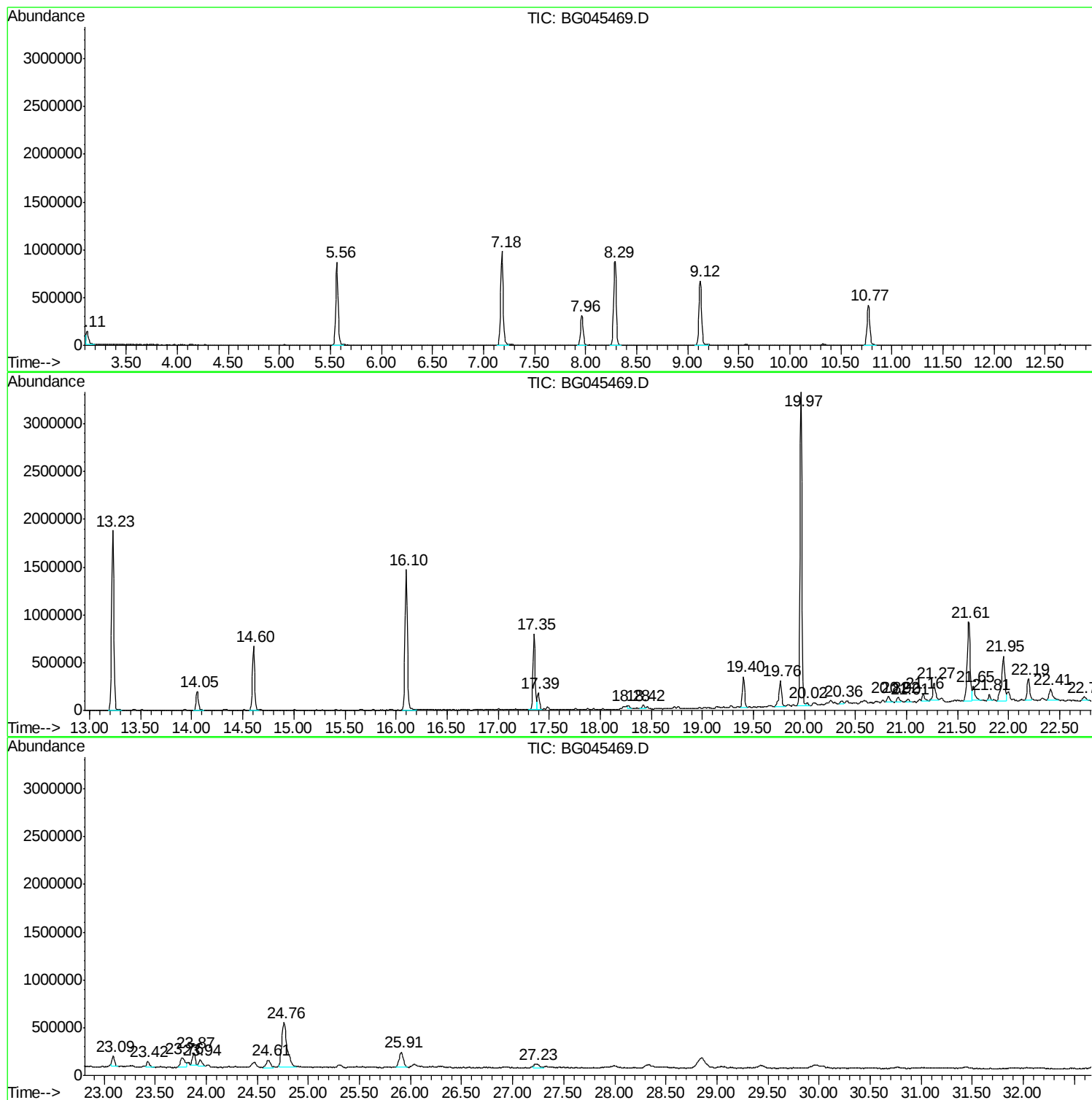
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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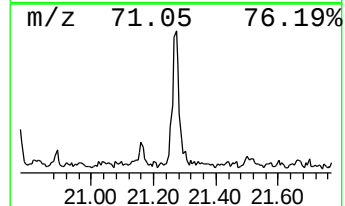
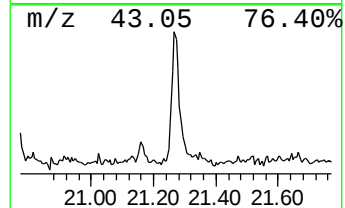
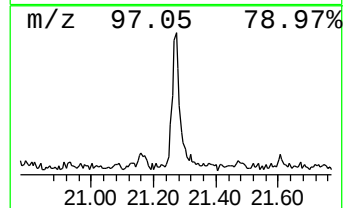
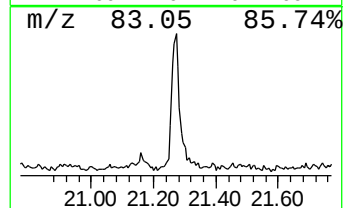
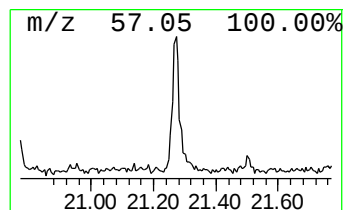
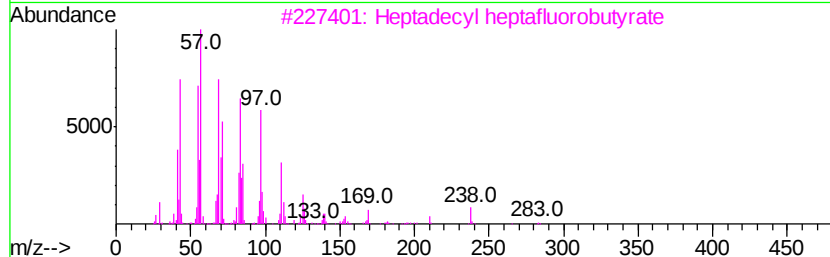
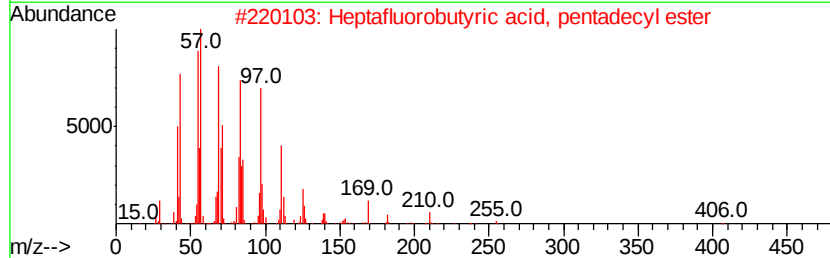
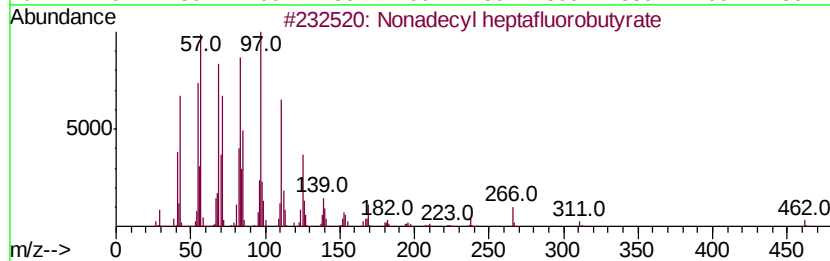
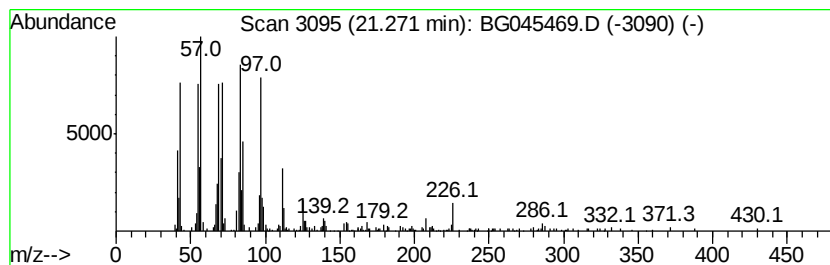
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Nonadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.27	3.83 ng	310017	Chrysene-d12	21.61	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecyl heptafluorobutvrate	480	C23H39F7O2	1000351-83-9	91
2	Heptafluorobutvric acid, pentade...	424	C19H31F7O2	959261-23-5	91
3	Heptadecyl heptafluorobutvrate	452	C21H35F7O2	959085-66-6	91
4	9-Nonadecene	266	C19H38	031035-07-1	90
5	1-Nonadecene	266	C19H38	018435-45-5	89



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Instrument :
BNA_G
ClientSampleId :
NM42-COMP-2020-0-6

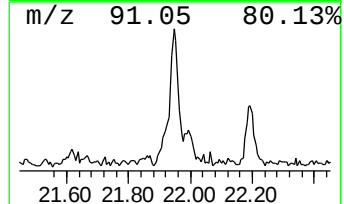
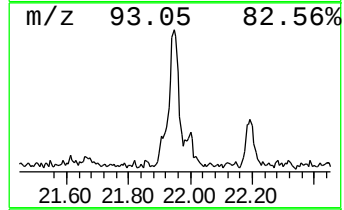
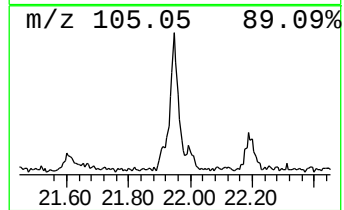
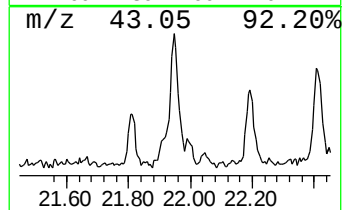
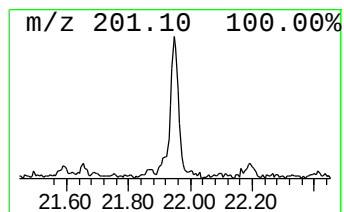
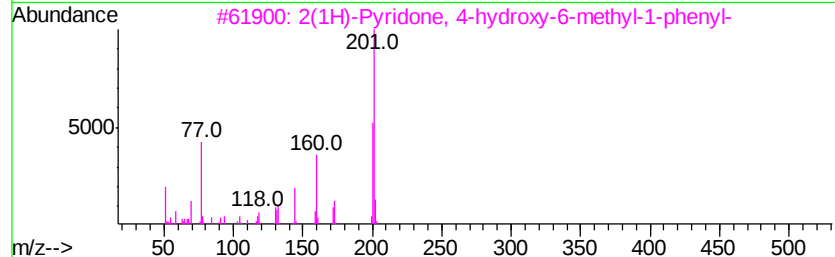
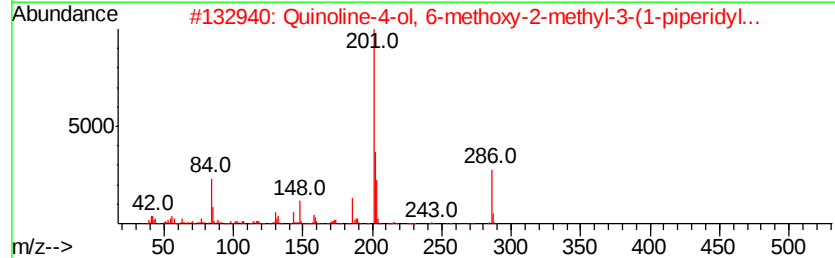
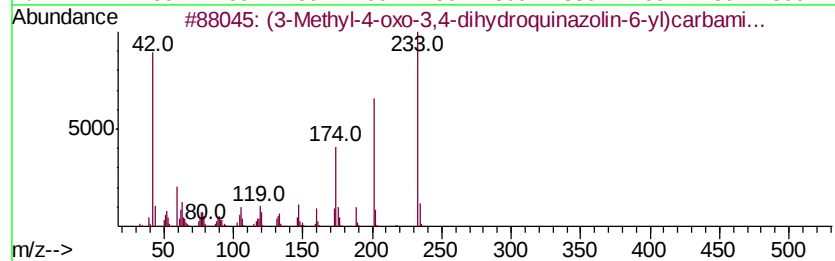
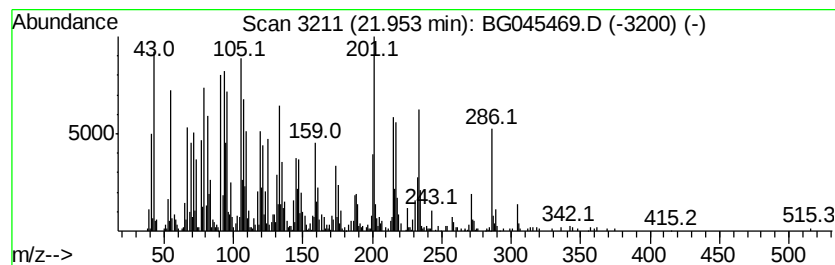
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Peak Number 4 unknown21.95 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.95	12.41 ng	1004310	Chrysene-d12	21.61

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		(3-Methyl-4-oxo-3,4-dihydroquina...	233	C11H11N3O3	1000309-93-7	25
2		Quinoline-4-ol, 6-methoxy-2-meth...	286	C17H22N2O2	309740-32-7	18
3		2(1H)-Pyrindone, 4-hydroxy-6-meth...	201	C12H11N02	015250-44-9	11
4		6-Trifluoromethylloxindole	201	C9H6F3N0	001735-89-3	11
5		1H-Inden-1-one, 5-(1,1-dimethyle...	216	C15H20O	038393-93-0	11



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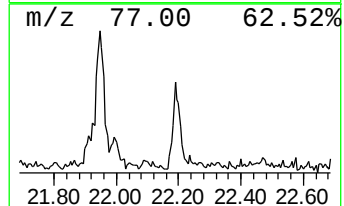
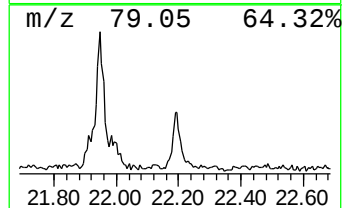
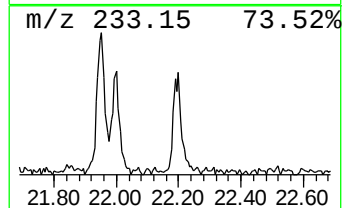
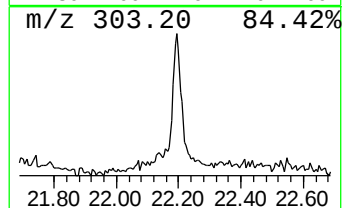
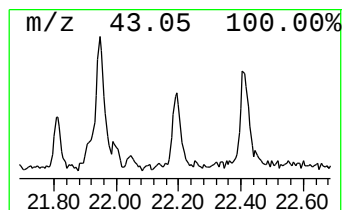
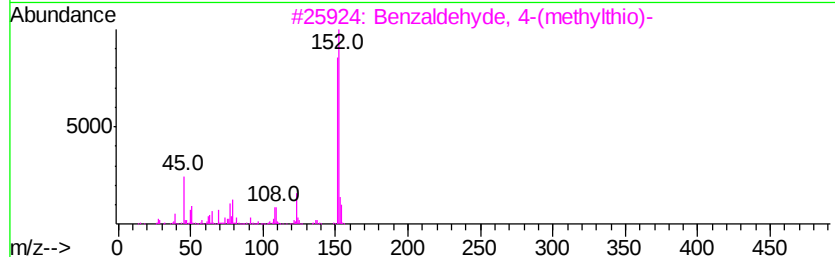
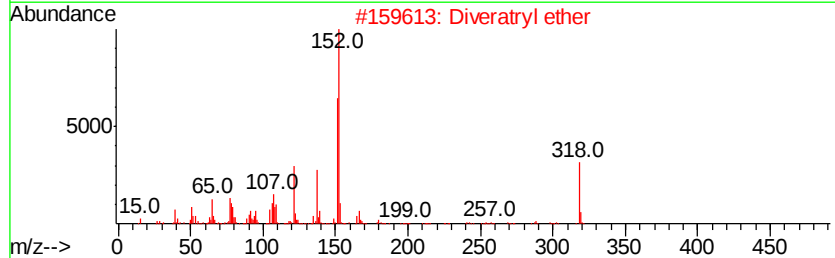
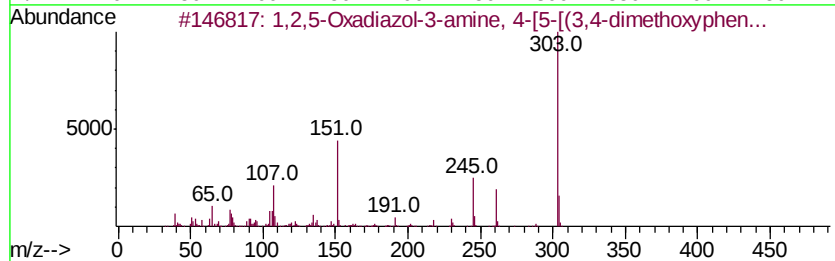
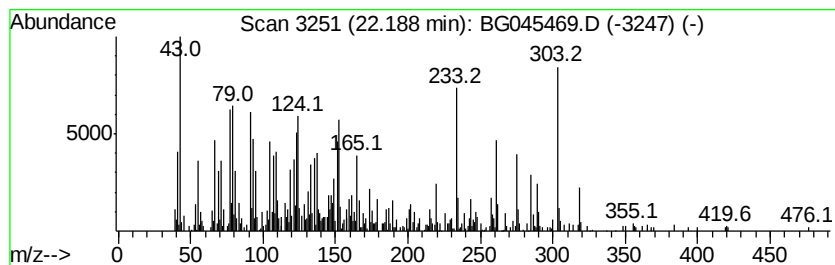
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG051520.M
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 unknown22.19 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.19	4.82 ng	390097	Chrysene-d12	21.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2,5-Oxadiazol-3-amine, 4-[5-[(...]	303	C13H13N5O4	1000337-43-2	35
2		Diveratryl ether	318	C18H22O5	023702-54-7	25
3		Benzaldehyde, 4-(methylthio)-	152	C8H8OS	003446-89-7	15
4		4-Amino-6-[2-naphthylthio]quinaz...	303	C18H13N3S	052979-15-4	15
5		Morphinan-3,6,14-triol, 4,5-epox...	303	C17H21NO4	054934-75-7	15



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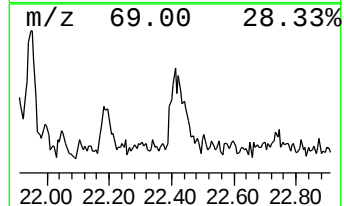
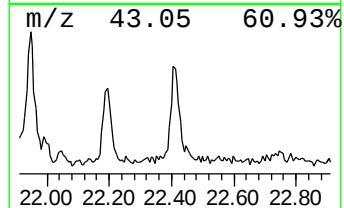
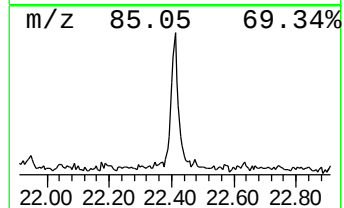
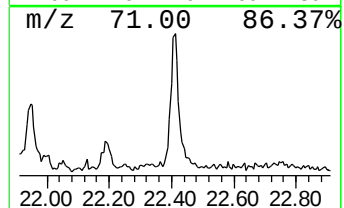
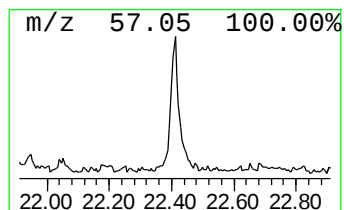
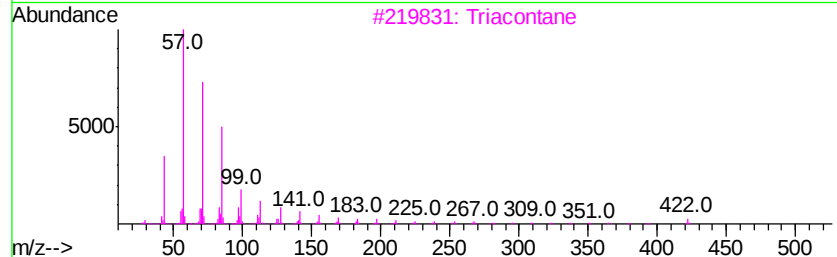
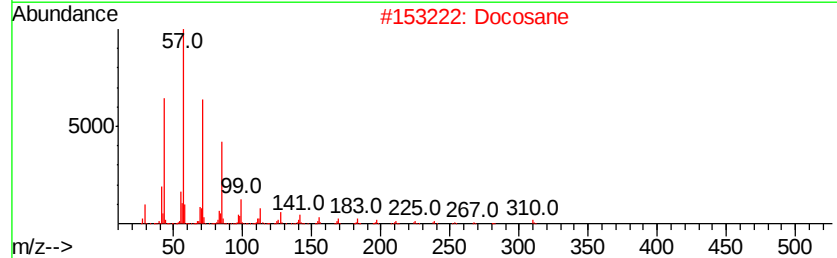
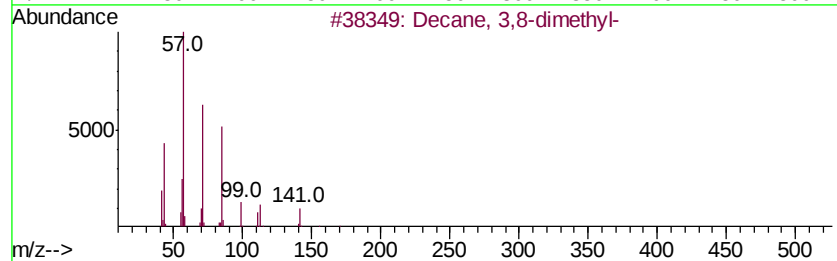
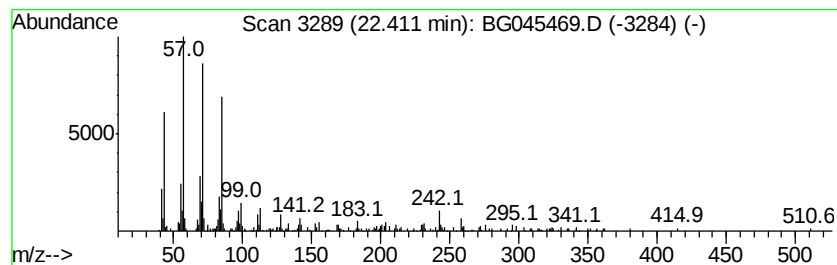
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Peak Number 6 Decane, 3,8-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.41	3.00 ng	242931	Chrysene-d12	21.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
2		Docosane	310	C22H46	000629-97-0	83
3		triacontane	422	C30H62	000638-68-6	83
4		Pentadecane	212	C15H32	000629-62-9	83
5		Hexacosane	366	C26H54	000630-01-3	80



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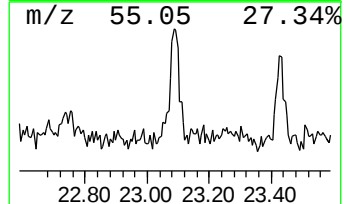
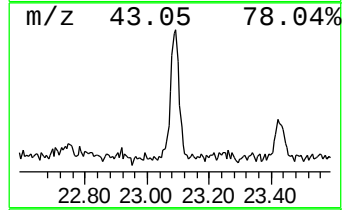
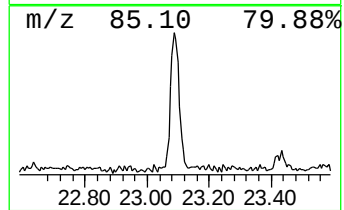
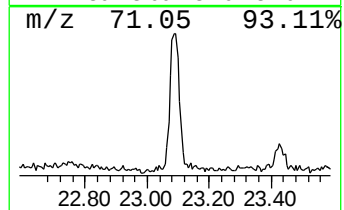
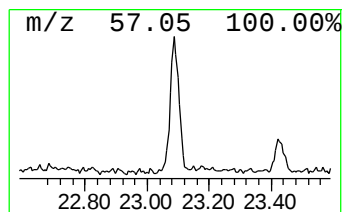
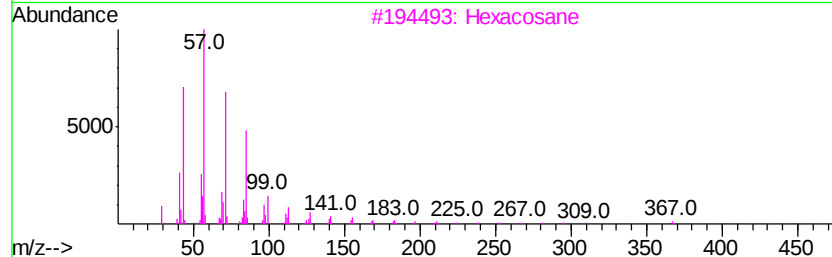
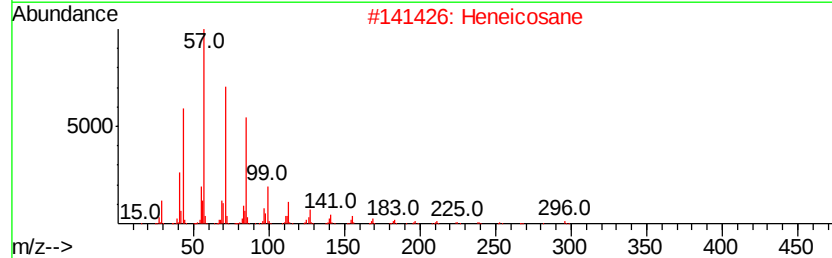
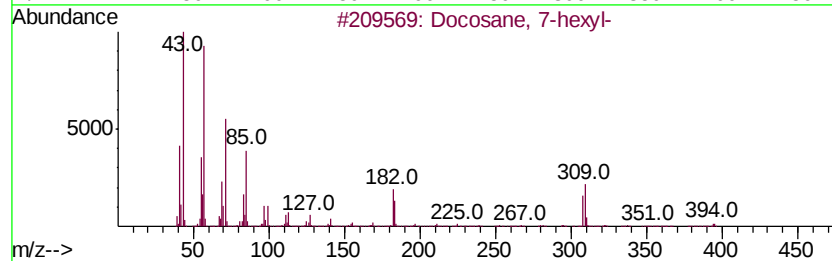
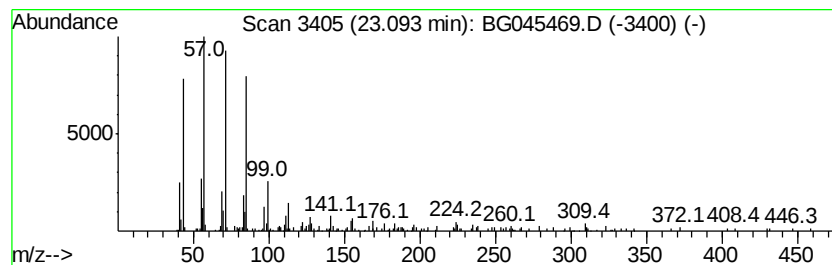
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Docosane, 7-hexyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.09	2.62 ng	211971	Chrysene-d12	21.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane, 7-hexyl-	394	C28H58	055373-86-9	93
2		Heneicosane	296	C21H44	000629-94-7	91
3		Hexacosane	366	C26H54	000630-01-3	87
4		Octacosane	394	C28H58	000630-02-4	86
5		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052620\
Data File : BG045469.D
Acq On : 26 May 2020 22:59
Operator : CG/JU
Sample : L2744-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NM42-COMP-2020-0-6

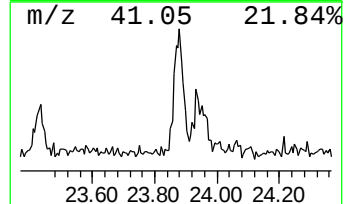
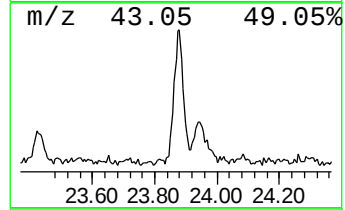
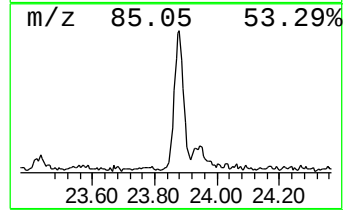
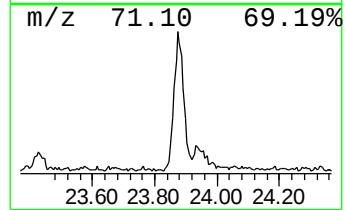
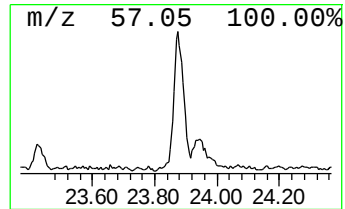
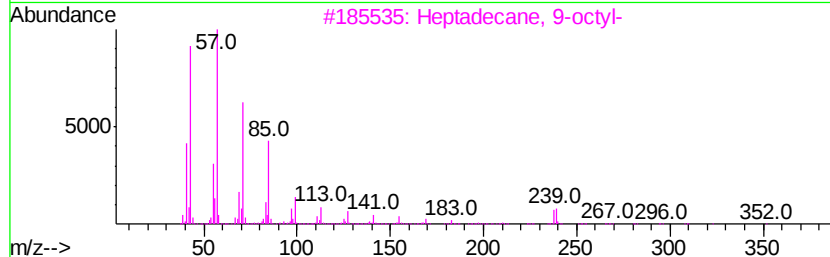
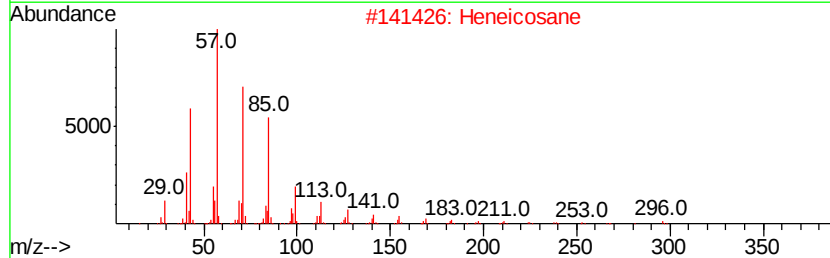
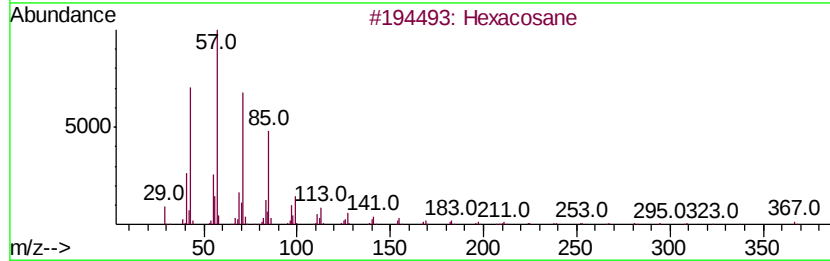
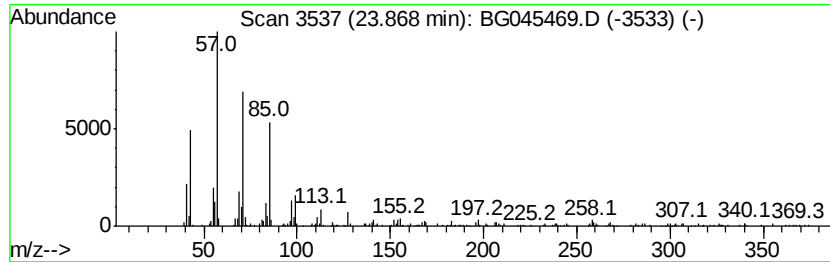
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.87	3.17 ng	258947	Perylene-d12	24.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	90
5		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052620\
Data File : BG045469.D
Acq On : 26 May 2020 22:59
Operator : CG/JU
Sample : L2744-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NM42-COMP-2020-0-6

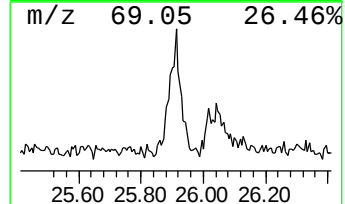
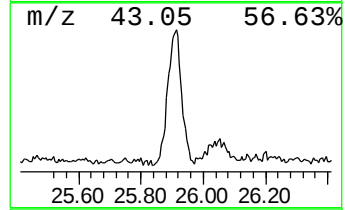
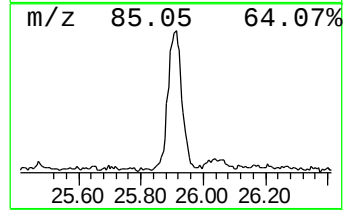
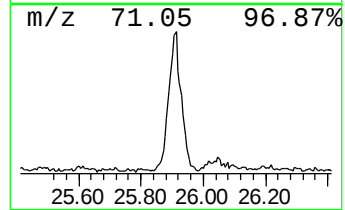
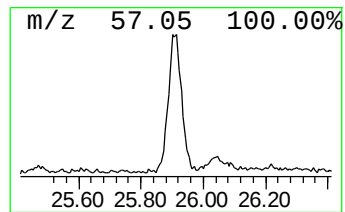
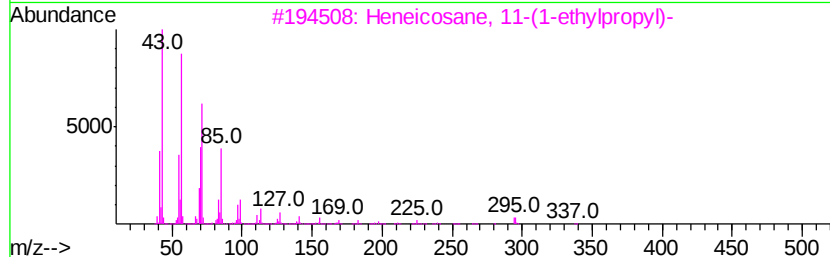
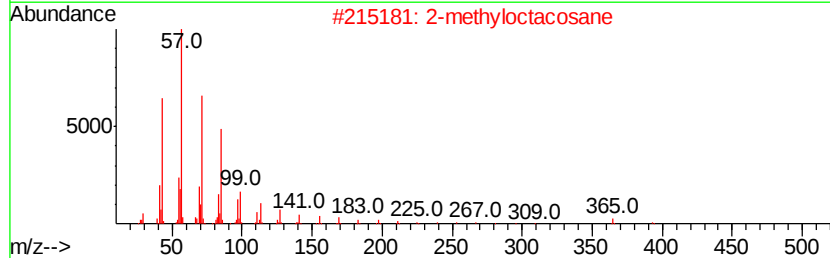
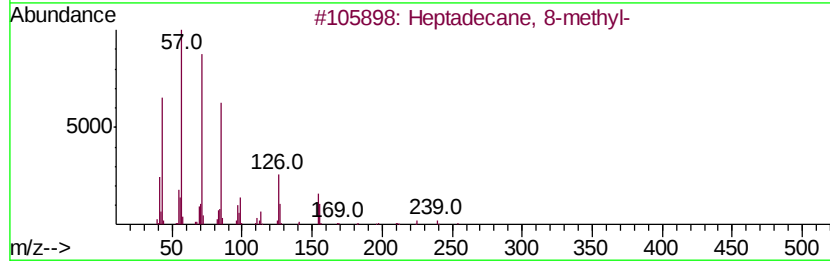
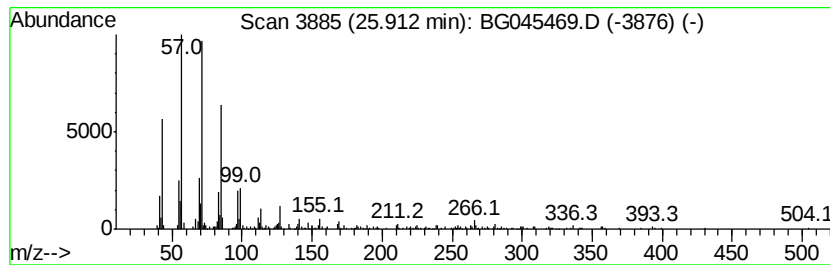
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane, 8-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.91	5.53 ng	452378	Perylene-d12	24.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	89
2		2-methyloctacosane	408	C29H60	1000376-72-8	87
3		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	80
4		Tetratetracontane	619	C44H90	007098-22-8	80
5		Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG052620\
Data File : BG045469.D
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Operator : CG/JU
Sample : L2744-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NM42-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.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
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unknown21.95	21.95	12.4 ng		1004310	5	21.61	1618130	20.0
unknown22.19	22.19	4.8 ng		390097	5	21.61	1618130	20.0
Decane, 3,8-dimet...	22.41	3.0 ng		242931	5	21.61	1618130	20.0
Docosane, 7-hexyl-	23.09	2.6 ng		211971	5	21.61	1618130	20.0
Hexacosane	23.87	3.2 ng		258947	6	24.76	1635820	20.0
Heptadecane, 8-me...	25.91	5.5 ng		452378	6	24.76	1635820	20.0