LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM090319\
Data File : BM022497.D
Acq On : 03 Sep 2019 11:38
Operator : HP/JU
Sample : K4619-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP1-COMP

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_M\METHODS\8270-BM082919.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	5.128	359	364	380	rBV	275568	406976	40.53%	7.177%
2	6.704	626	632	645	rBV	241981	423576	42.19%	7.470%
3	7.039	684	689	702	rBV	302971	481449	47.95%	8.490%
4	7.504	763	768	775	rBB	83850	123396	12.29%	2.176%
5	7.816	815	821	831	rBB	245425	387222	38.56%	6.829%
6	8.681	962	968	989	rBV	123923	263003	26.19%	4.638%
7	10.286	1235	1241	1257	rBV	60805	130762	13.02%	2.306%
8	12.774	1658	1664	1683	rBV	357663	598579	59.61%	10.556%
9	13.663	1810	1815	1825	rBB	17793	29421	2.93%	0.519%
10	14.174	1896	1902	1913	rBB2	100326	168951	16.83%	2.979%
11	15.686	2154	2159	2176	rBB	292233	508366	50.63%	8.965%
12	16.945	2368	2373	2389	rBV	97883	180590	17.99%	3.185%
13	17.833	2519	2524	2535	rBV2	61147	94180	9.38%	1.661%
14	19.003	2721	2723	2735	rVB4	10729	17697	1.76%	0.312%
15	19.127	2739	2744	2754	rBV2	28698	51264	5.11%	0.904%
16	19.580	2816	2821	2832	rBV	811576	1004084	100.00%	17.707%
17	20.215	2926	2929	2934	rVB2	26606	29007	2.89%	0.512%
18	20.850	3032	3037	3045	rBV2	42560	67697	6.74%	1.194%
19	21.162	3086	3090	3098	rBV	136230	222210	22.13%	3.919%
20	21.280	3108	3110	3113	rBV4	10053	11639	1.16%	0.205%
21	21.703	3179	3182	3186	rBV	21939	28292	2.82%	0.499%
22	22.150	3255	3258	3263	rVB	31910	36856	3.67%	0.650%
23	22.633	3336	3340	3346	rBV2	48947	64554	6.43%	1.138%
24	23.168	3427	3431	3438	rVB3	46020	67667	6.74%	1.193%
25	23.350	3457	3462	3472	rBV	109483	217923	21.70%	3.843%
26	23.774	3531	3534	3541	rVB	35484	55303	5.51%	0.975%

Sum of corrected areas: 5670664

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM090319\
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Sample : K4619-03
Misc :
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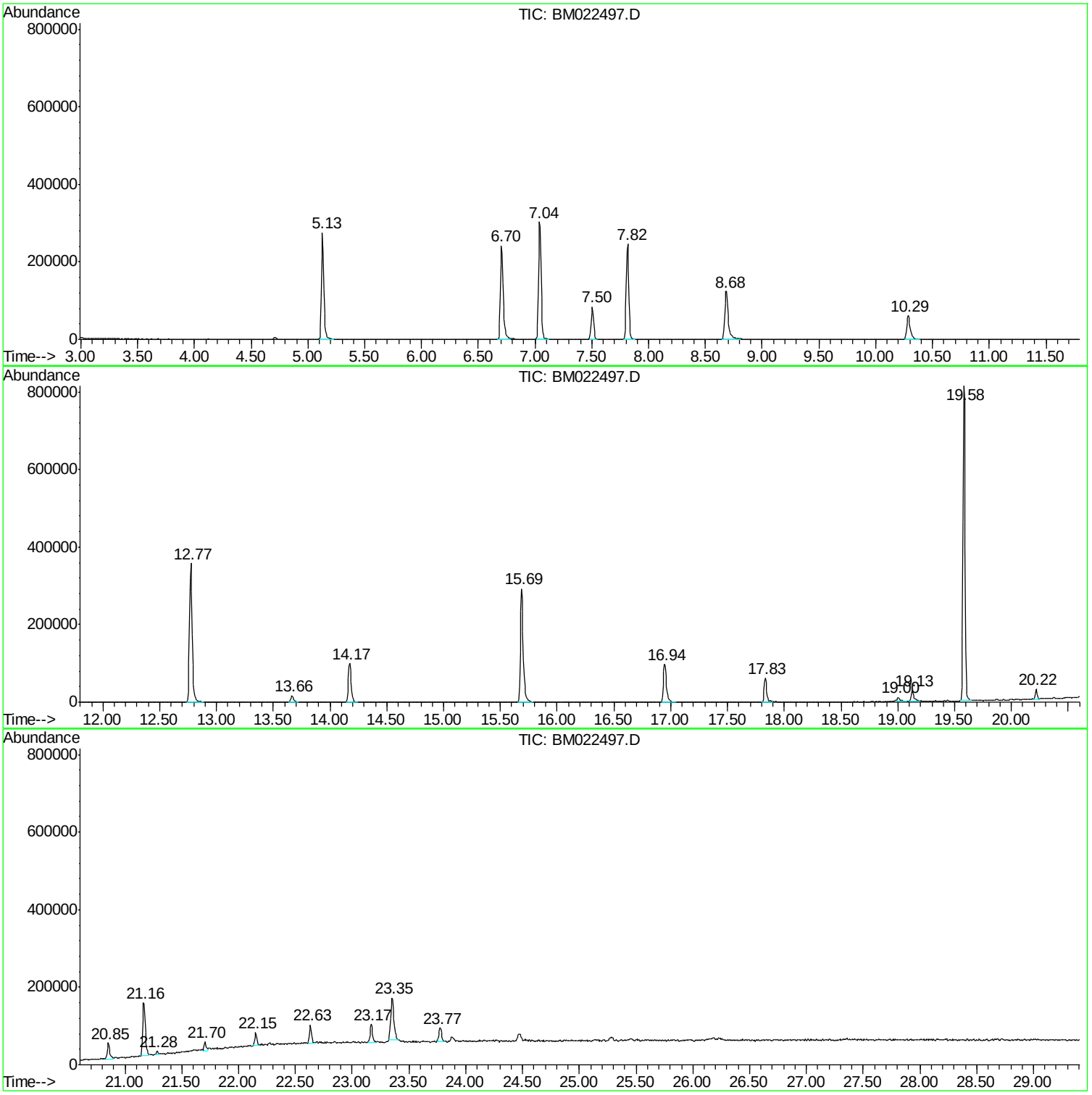
Instrument : BNA_M
ClientSampleId : TP1-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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TIC Library : C:\DATABASE\NIST11.L
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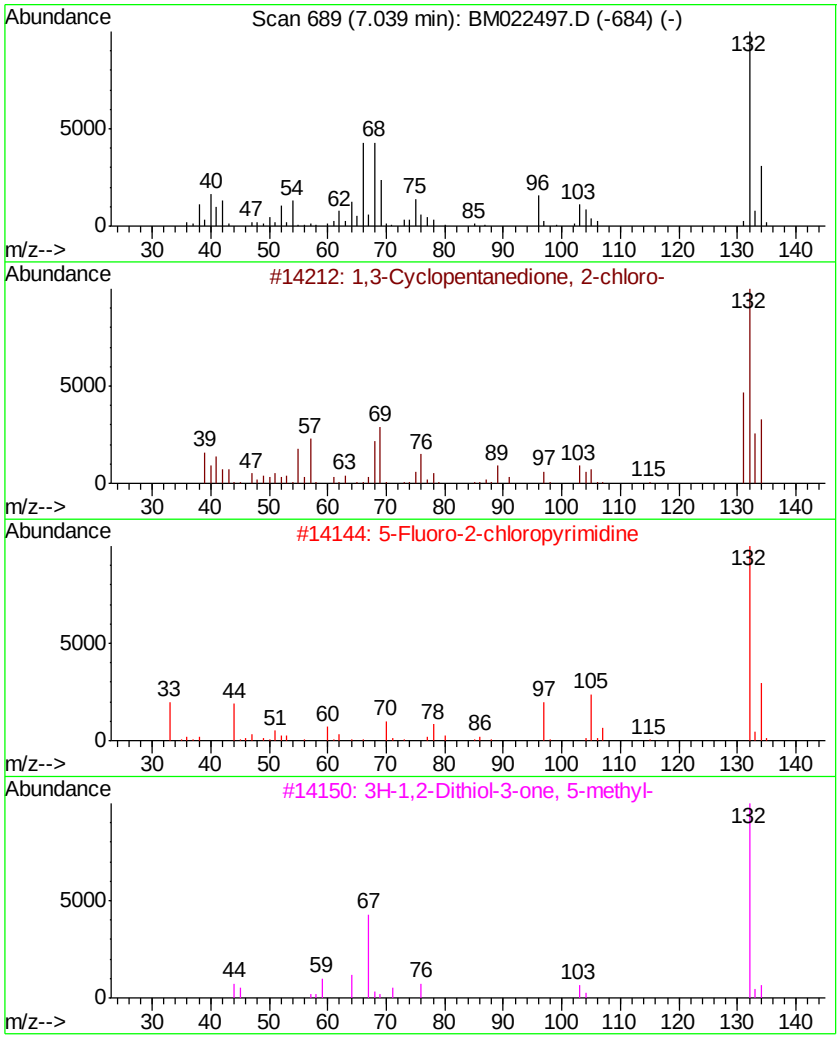
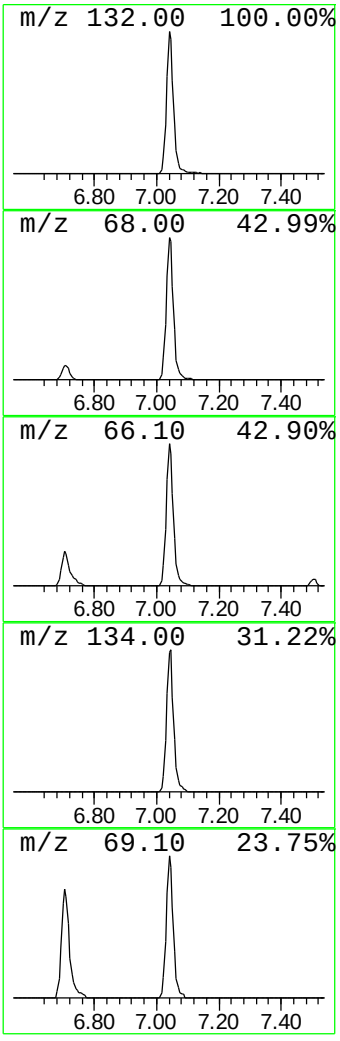
Peak Number 1 unknown7.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.04	78.03 ng	481449	1,4-Dichlorobenzene-d4	7.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	16
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
3	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
4	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14





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Instrument : BNA_M
ClientSampleId : TP1-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.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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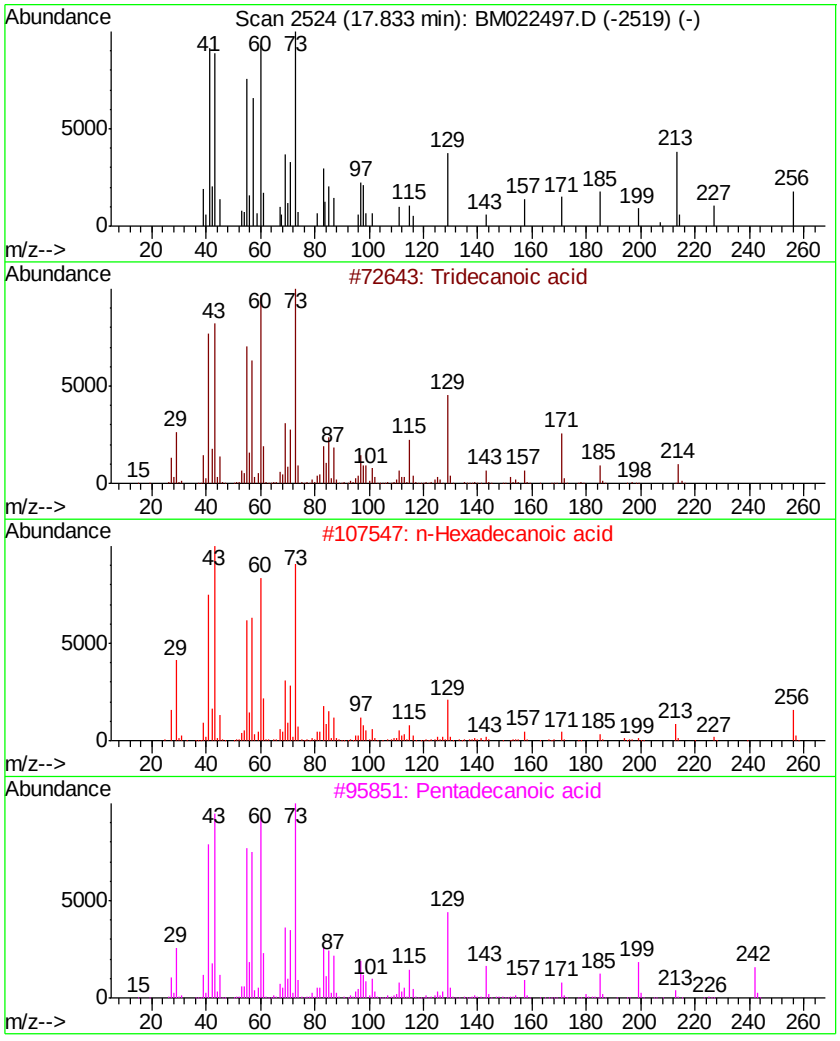
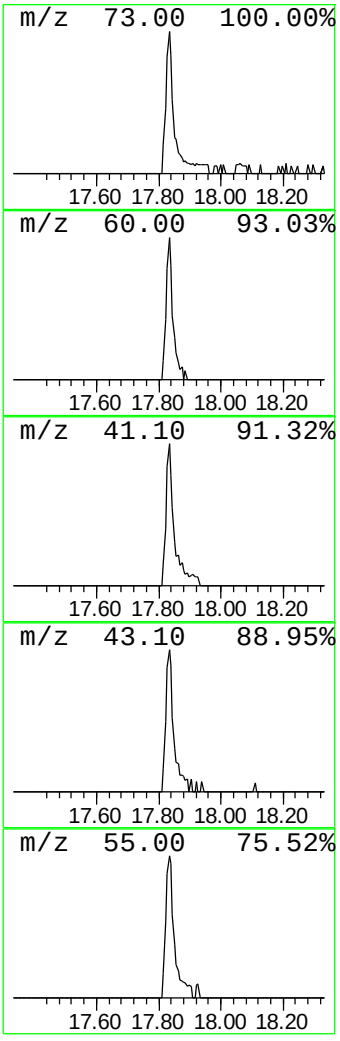
Peak Number 3 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.83	10.43 ng	94180	Phenanthrene-d10	16.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	64
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
5	n-Decanoic acid	172	C10H20O2	000334-48-5	43





Library Search Compound Report

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Data File : BM022497.D
Acq On : 03 Sep 2019 11:38
Operator : HP/JU
Sample : K4619-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP1-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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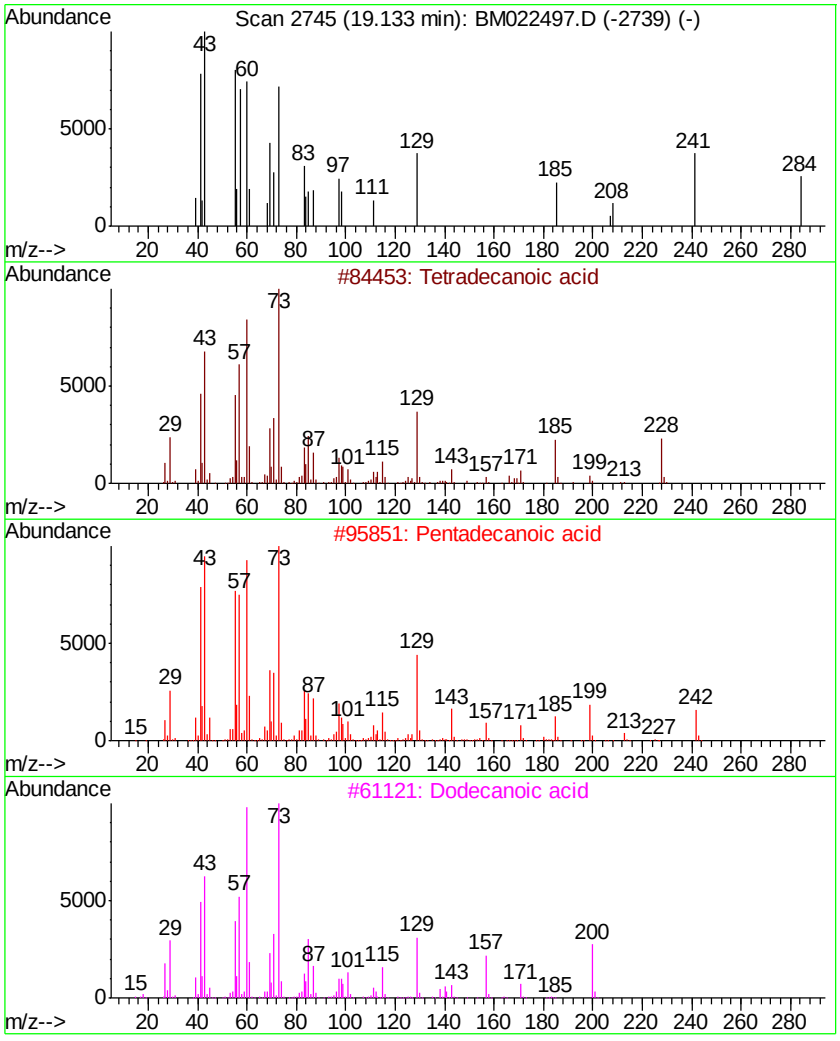
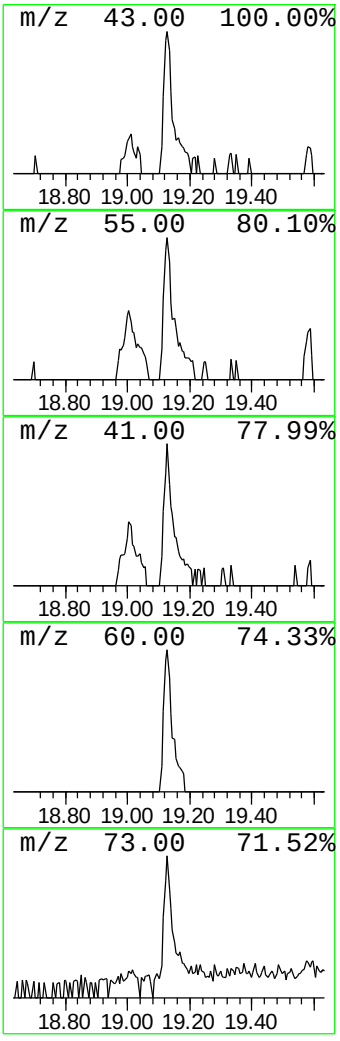
Peak Number 4 Tetradecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.13	4.61 ng	51264	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	49
3	Dodecanoic acid	200	C12H24O2	000143-07-7	43
4	Undecanoic acid	186	C11H22O2	000112-37-8	43
5	Tridecanoic acid	214	C13H26O2	000638-53-9	43





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Operator : HP/JU
Sample : K4619-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP1-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.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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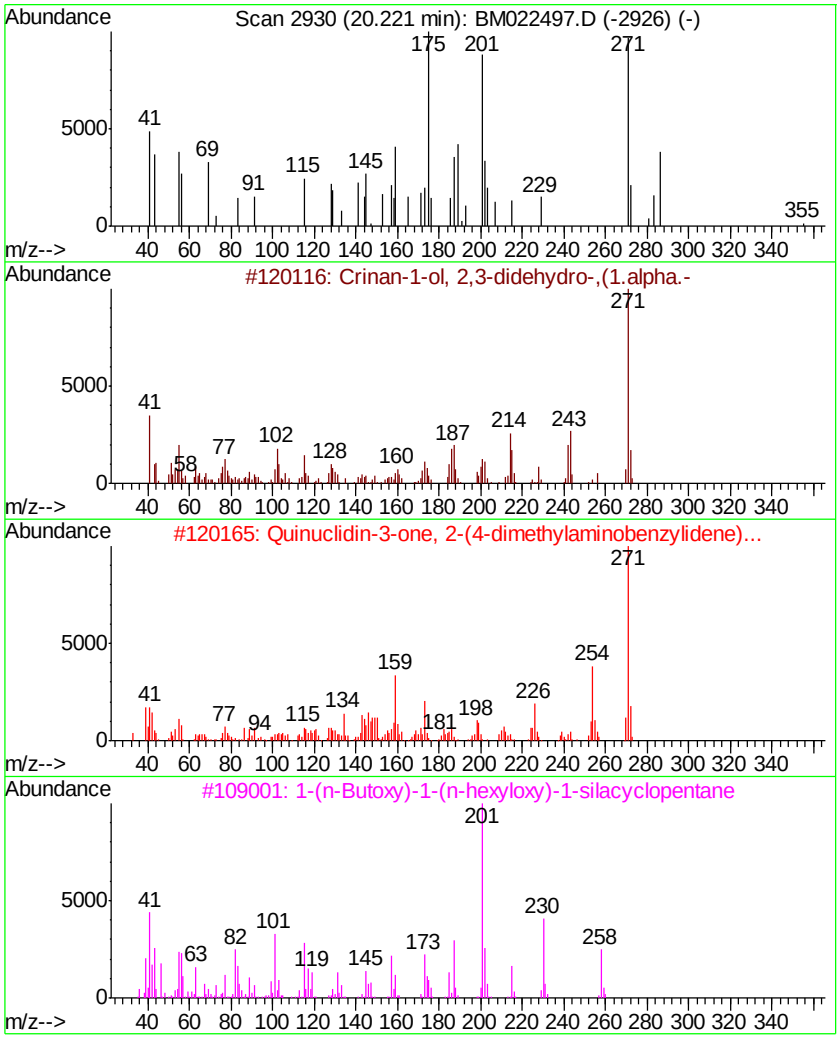
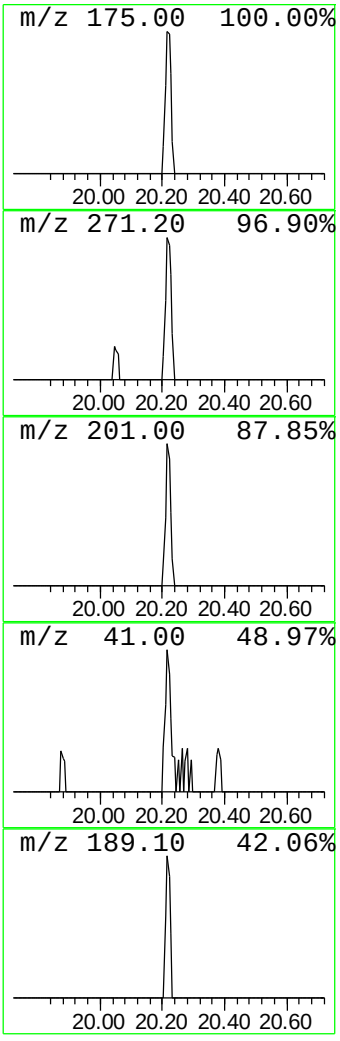
Peak Number 5 unknown20.22 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.22	2.61 ng	29007	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Crinan-1-ol, 2,3-didehydro-,(1.a...	271	C16H17NO3	1000111-31-3	14
2	Quinuclidin-3-one, 2-(4-dimethyl...	271	C16H21N3O	1000266-14-6	14
3	1-(n-Butoxy)-1-(n-hexyloxy)-1-si...	258	C14H30O2Si	1000245-75-4	14
4	Silane, dimethyl(3-methylbut-2-e...	286	C16H34O2Si	1000347-96-9	12
5	4'-Azidobenzo[1',2'-b]-1,4-diaza...	201	C10H11N5	120287-75-4	10





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Misc :
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Instrument : BNA_M
ClientSampleId : TP1-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.M
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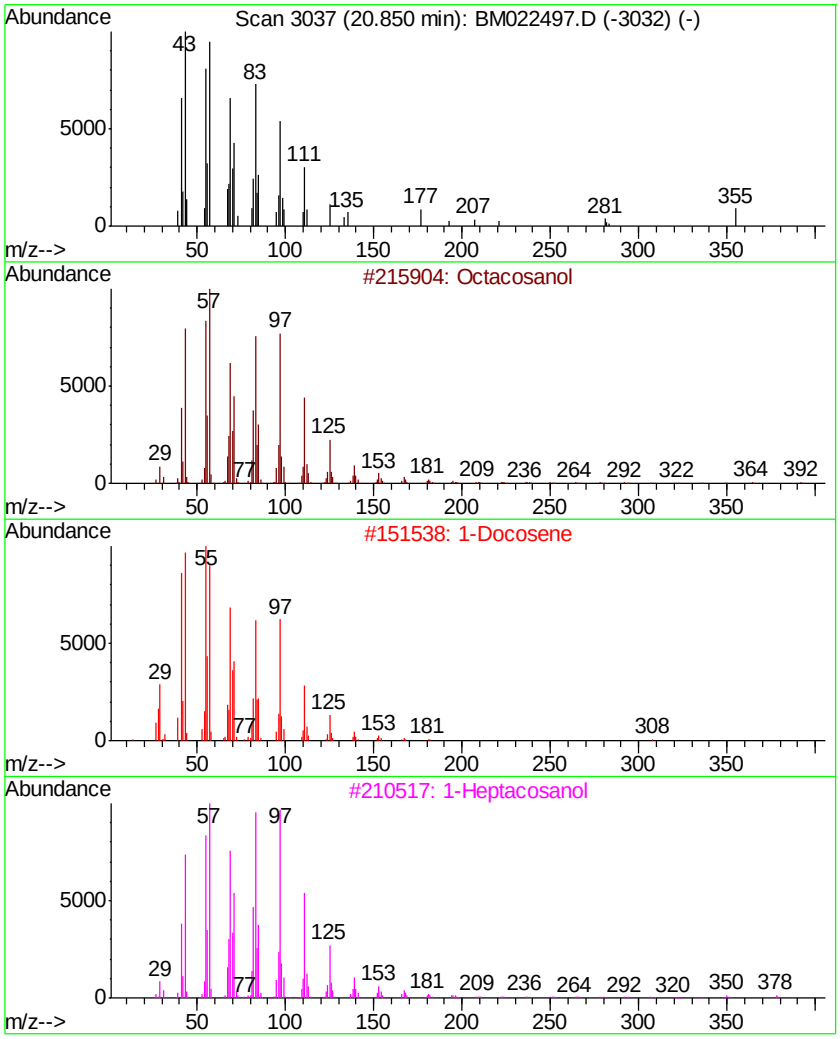
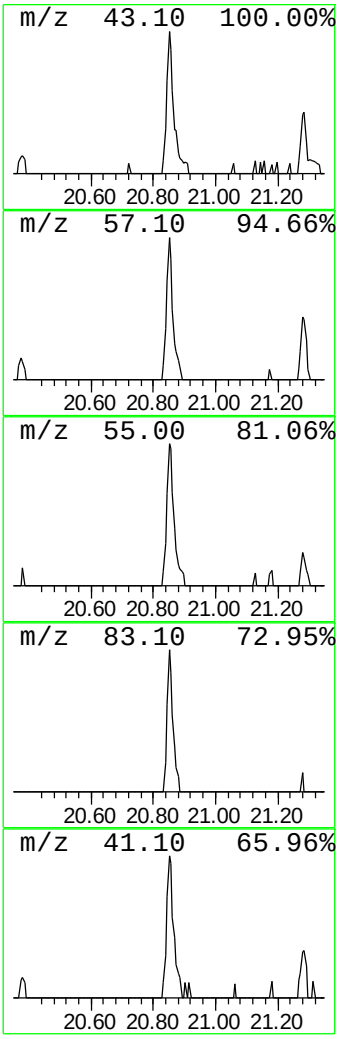
Peak Number 6 Octacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.85	6.09 ng	67697	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	90
2	1-Docosene	308	C22H44	001599-67-3	90
3	1-Heptacosanol	396	C27H56O	002004-39-9	90
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
5	1-Tricosene	322	C23H46	018835-32-0	90





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Instrument : BNA_M
ClientSampleId : TP1-COMP

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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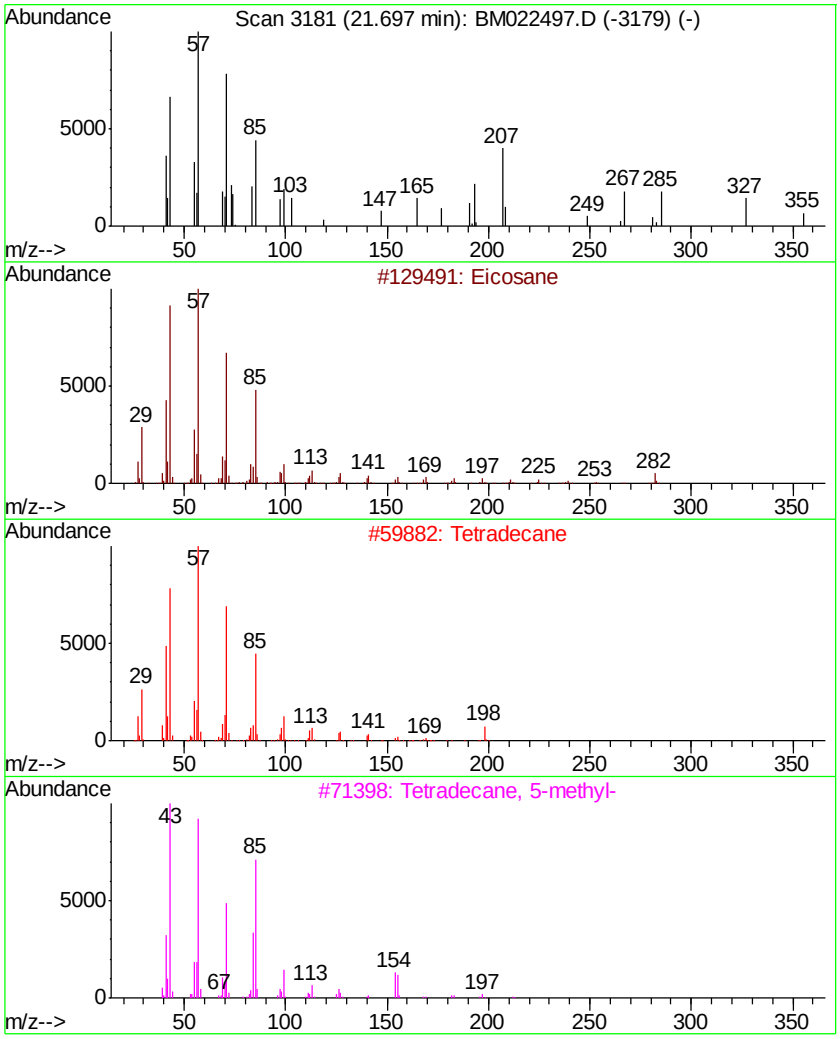
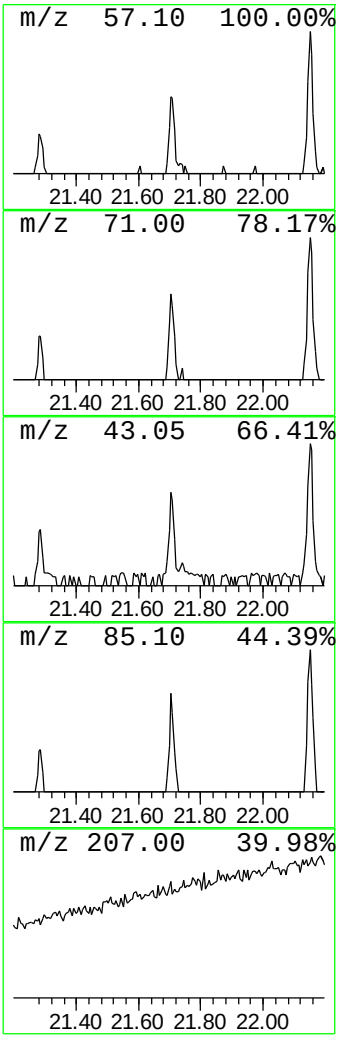
Peak Number 7 unknown21.70 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.70	2.55 ng	28292	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	45
2	Tetradecane	198	C14H30	000629-59-4	35
3	Tetradecane, 5-methyl-	212	C15H32	025117-32-2	35
4	Hexadecane	226	C16H34	000544-76-3	35
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	35





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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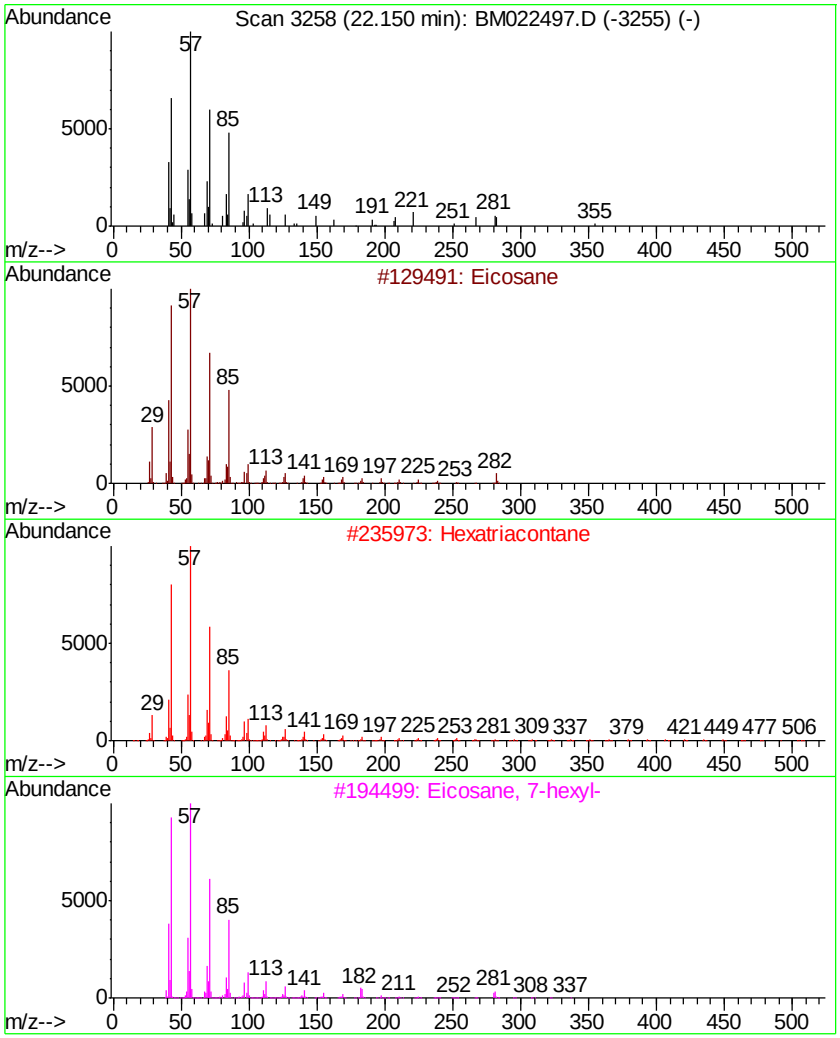
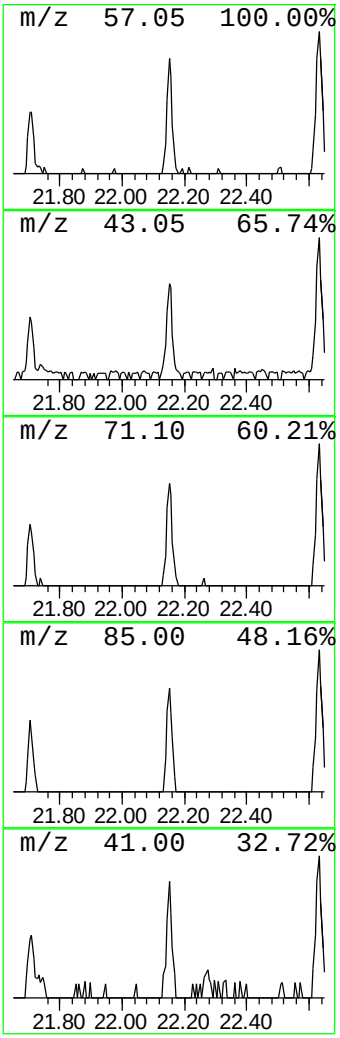
Peak Number 8 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.15	3.32 ng	36856	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Hexatriacontane	507	C36H74	000630-06-8	80
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	80
4	Octacosane	394	C28H58	000630-02-4	80
5	Heptadecane	240	C17H36	000629-78-7	80





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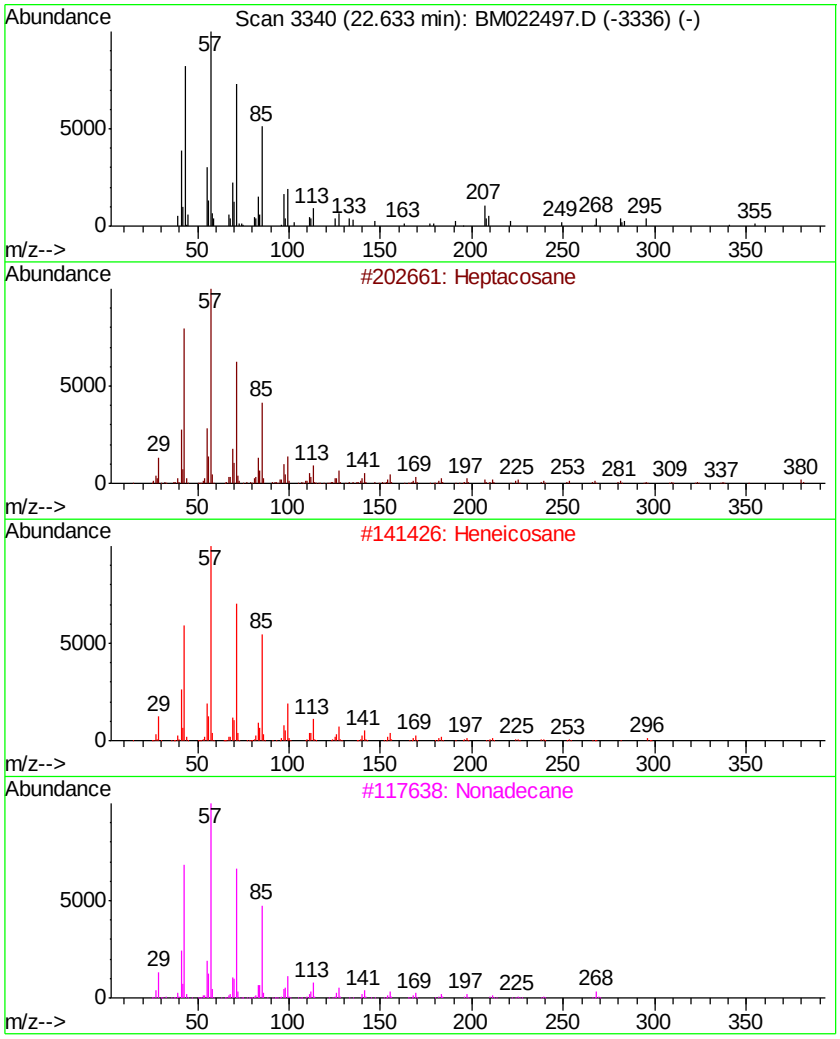
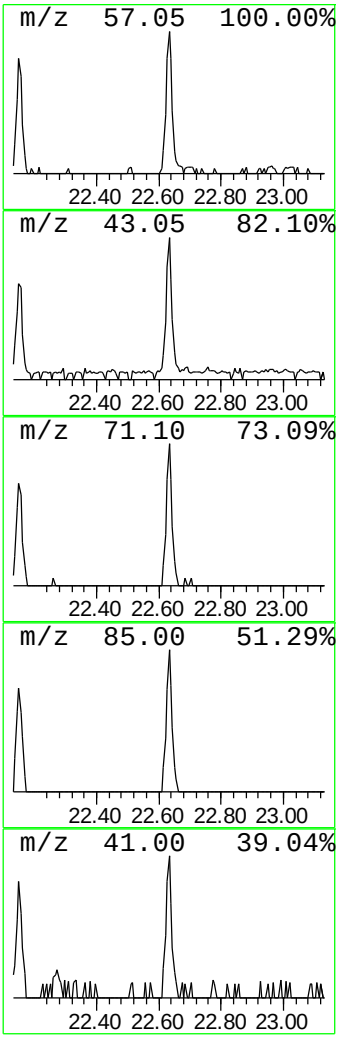
Peak Number 9 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.63	5.92 ng	64554	Perylene-d12	23.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	72
2	Heneicosane	296	C21H44	000629-94-7	64
3	Nonadecane	268	C19H40	000629-92-5	64
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	64
5	Eicosane	282	C20H42	000112-95-8	62





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TIC Library : C:\DATABASE\NIST11.L
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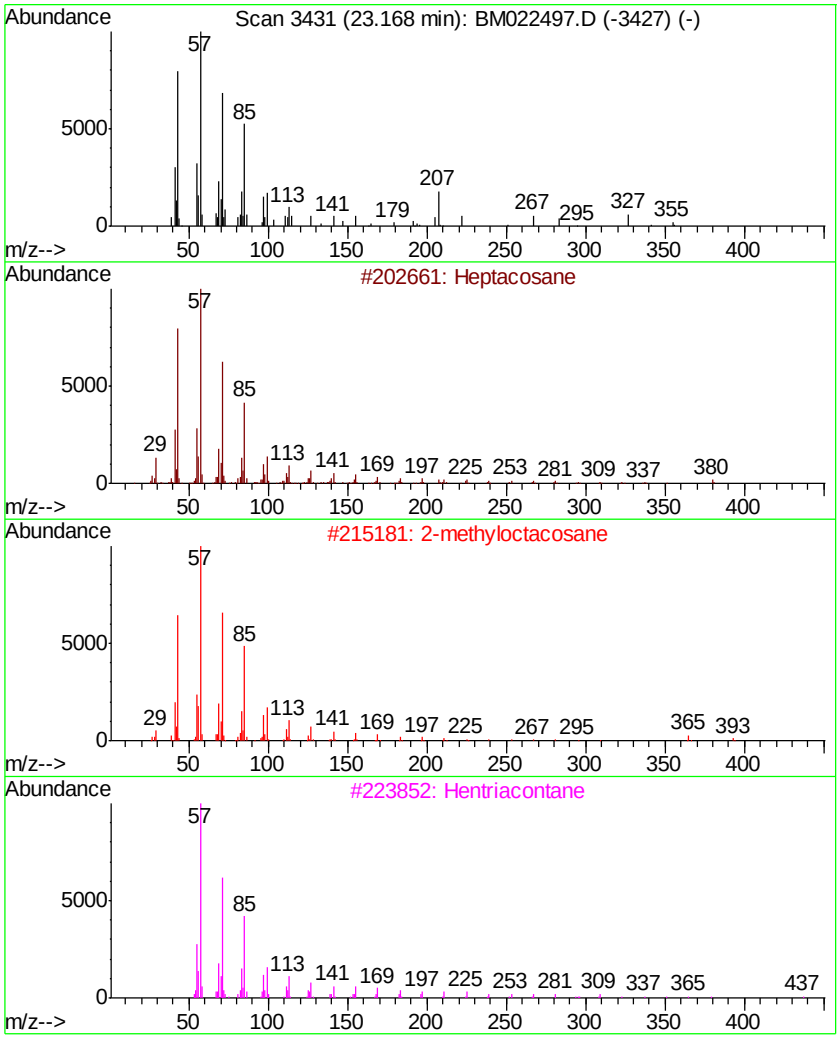
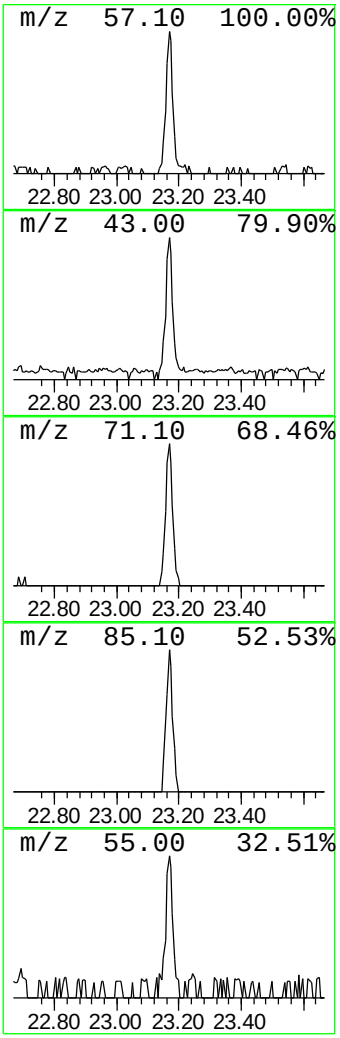
Peak Number 10 2-methyloctacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.17	6.21 ng	67667	Perylene-d12	23.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	83
2	2-methyloctacosane	408	C29H60	1000376-72-8	83
3	Hentriacontane	437	C31H64	000630-04-6	83
4	Hexacosane	366	C26H54	000630-01-3	83
5	Octacosane	394	C28H58	000630-02-4	80





Library Search Compound Report

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Misc :
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Instrument : BNA_M
ClientSampleId : TP1-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.M
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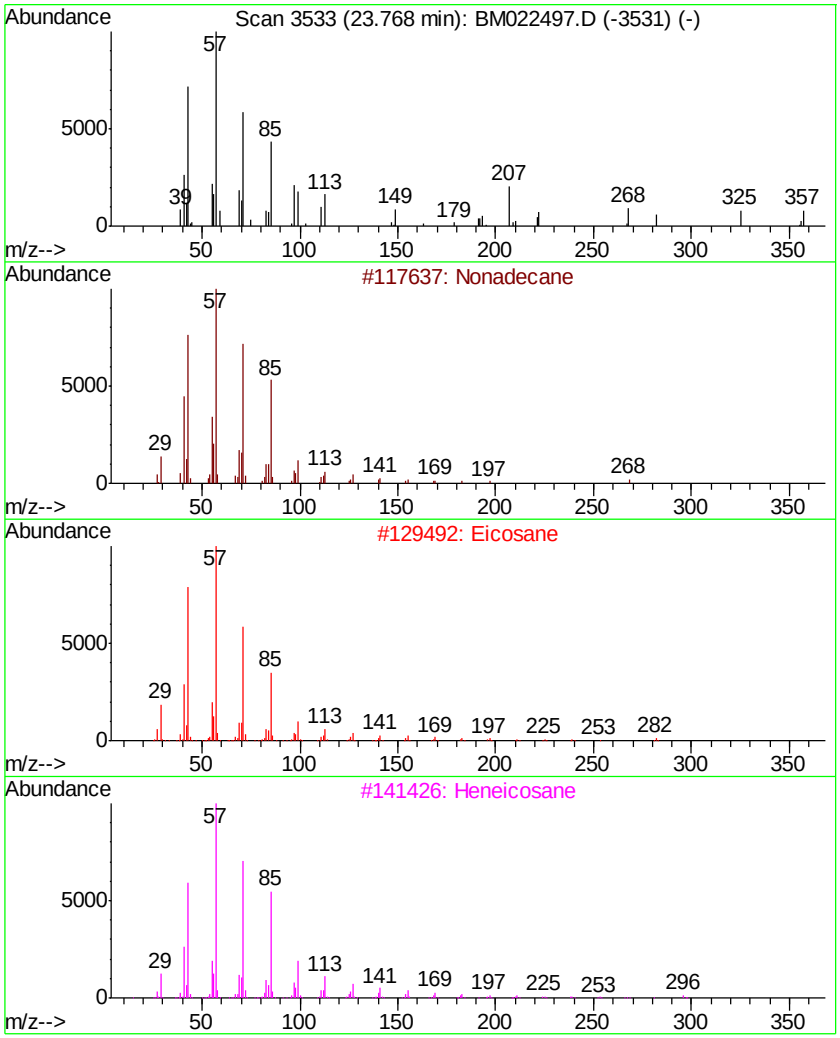
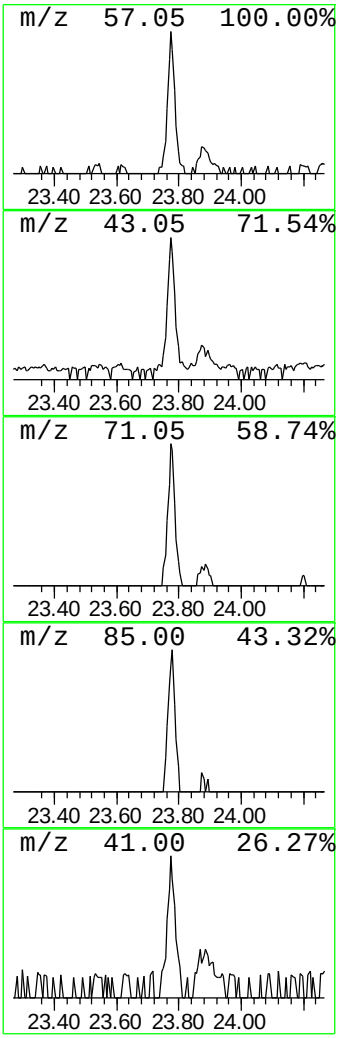
Peak Number 11 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.77	5.08 ng	55303	Perylene-d12	23.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	87
2	Eicosane	282	C20H42	000112-95-8	81
3	Heneicosane	296	C21H44	000629-94-7	80
4	Hentriacontane	437	C31H64	000630-04-6	80
5	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM090319\
Data File : BM022497.D
Acq On : 03 Sep 2019 11:38
Operator : HP/JU
Sample : K4619-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP1-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown7.04	7.04	78.0	ng	481449	1	7.50	123396	20.0
Tridecanoic acid	17.83	10.4	ng	94180	4	16.94	180590	20.0
Tetradecanoic acid	19.13	4.6	ng	51264	5	21.16	222210	20.0
unknown20.22	20.22	2.6	ng	29007	5	21.16	222210	20.0
Octacosanol	20.85	6.1	ng	67697	5	21.16	222210	20.0
unknown21.70	21.70	2.5	ng	28292	5	21.16	222210	20.0
Eicosane	22.15	3.3	ng	36856	5	21.16	222210	20.0
Heptacosane	22.63	5.9	ng	64554	6	23.35	217923	20.0
2-methyloctacosane	23.17	6.2	ng	67667	6	23.35	217923	20.0
Nonadecane	23.77	5.1	ng	55303	6	23.35	217923	20.0