LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052522\
Data File : BM035241.D
Acq On : 25 May 2022 14:03
Operator : CG/JU
Sample : N2978-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-303-20220519

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-BM042722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM035241.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.469	398	405	416	rBV	763090	1102074	17.94%	3.148%
2	7.057	669	675	686	rBV	392083	657399	10.70%	1.878%
3	7.887	808	816	825	rBV	354507	555759	9.04%	1.588%
4	9.046	1006	1013	1025	rBV	1061359	1787708	29.09%	5.107%
5	10.693	1285	1293	1301	rBV	413635	712917	11.60%	2.037%
6	13.151	1704	1711	1721	rBV	2757245	4045740	65.84%	11.558%
7	14.528	1938	1945	1953	rBV	638839	928926	15.12%	2.654%
8	16.016	2192	2198	2206	rBV	2227902	3093762	50.35%	8.838%
9	16.674	2307	2310	2320	rVB4	60247	122764	2.00%	0.351%
10	17.269	2405	2411	2419	rBV	769456	1106490	18.01%	3.161%
11	18.174	2560	2565	2580	rBV	642134	984062	16.01%	2.811%
12	18.451	2607	2612	2617	rBV2	84408	164127	2.67%	0.469%
13	18.504	2617	2621	2631	rVB	96387	181988	2.96%	0.520%
14	19.045	2709	2713	2718	rBV	53066	77855	1.27%	0.222%
15	19.121	2723	2726	2731	rVB2	144354	184802	3.01%	0.528%
16	19.257	2746	2749	2754	rBV	61019	70025	1.14%	0.200%
17	19.357	2763	2766	2771	rVB3	50130	63196	1.03%	0.181%
18	19.451	2778	2782	2791	rBV	478645	691041	11.25%	1.974%
19	19.798	2831	2841	2852	rBV2	222685	625927	10.19%	1.788%
20	19.898	2852	2858	2863	rBV	5240120	6144771	100.00%	17.554%
21	21.051	3048	3054	3062	rVB	361800	719637	11.71%	2.056%
22	21.174	3068	3075	3084	rBV	457961	1082348	17.61%	3.092%
23	21.451	3118	3122	3128	rBV	1096251	1450681	23.61%	4.144%
24	21.792	3176	3180	3190	rVB5	226694	510682	8.31%	1.459%
25	22.009	3212	3217	3230	rVB	185352	509261	8.29%	1.455%
26	23.833	3521	3527	3532	rBV2	771406	1562691	25.43%	4.464%
27	23.921	3533	3542	3568	rVB4	1139773	5867902	95.49%	16.763%

Sum of corrected areas: 35004535

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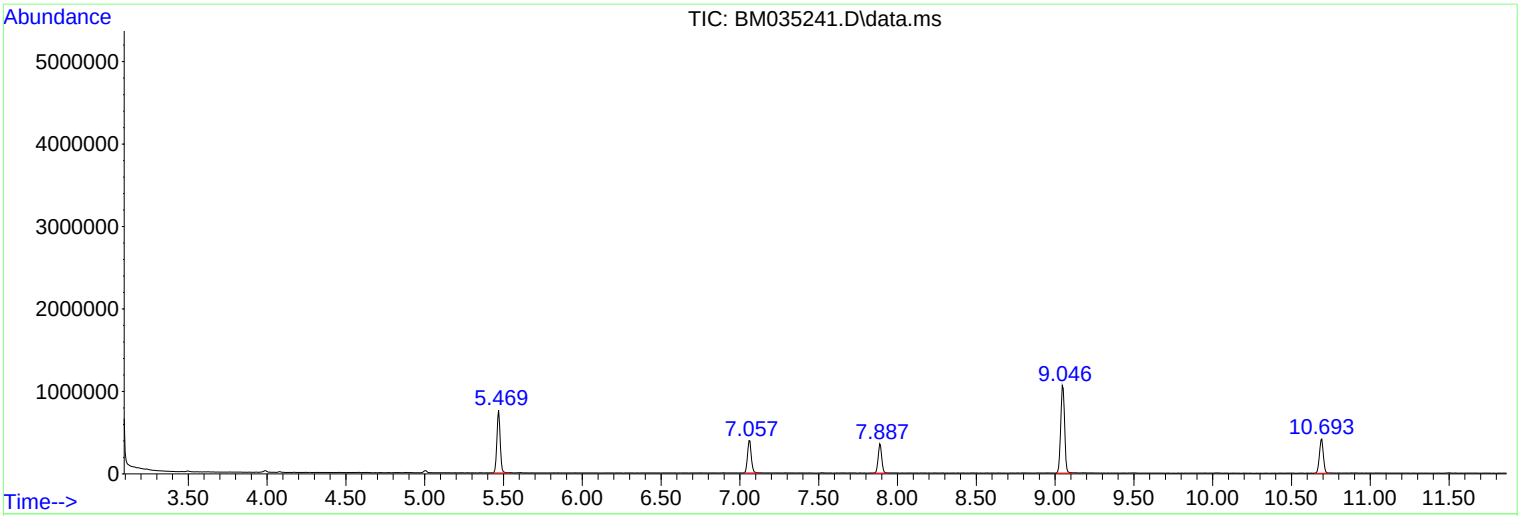
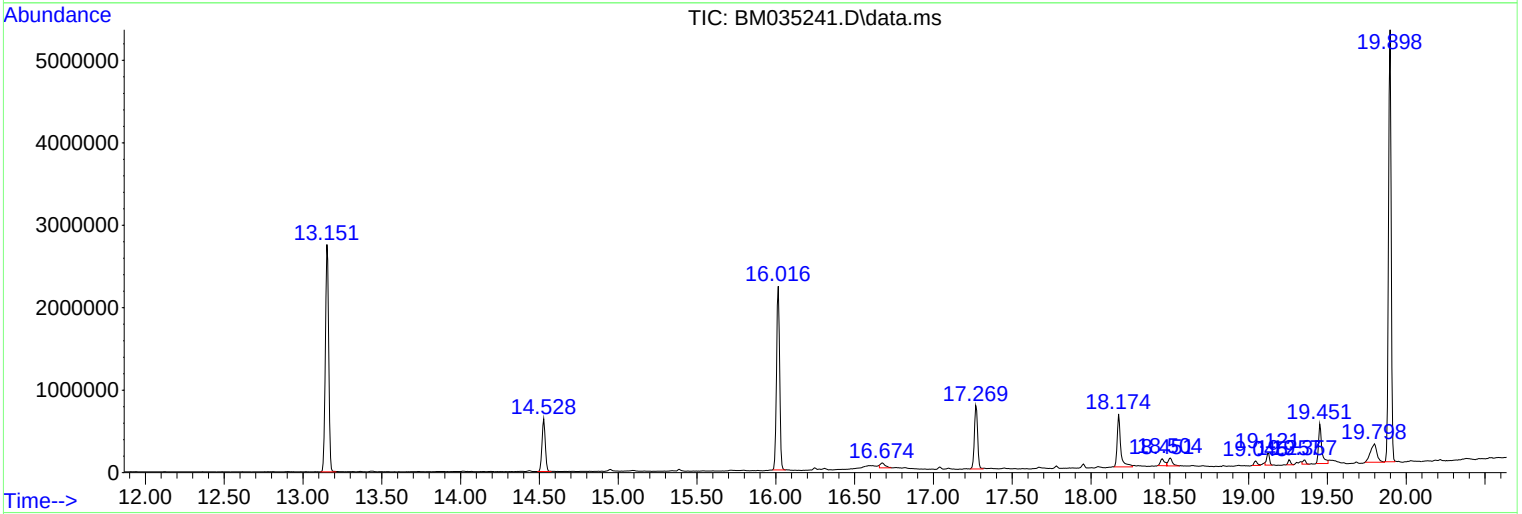
Misc :
ALS Vial : 8 Sample Multiplier: 1

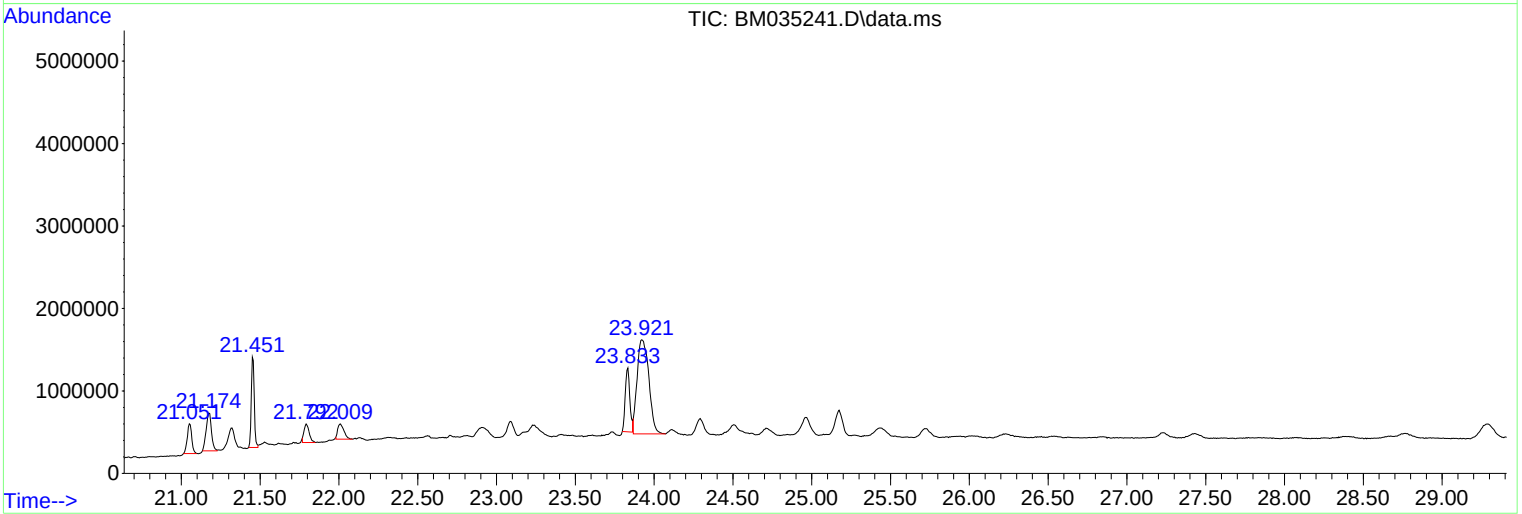
Instrument :
BNA_M
ClientSampleId :
SP-303-20220519

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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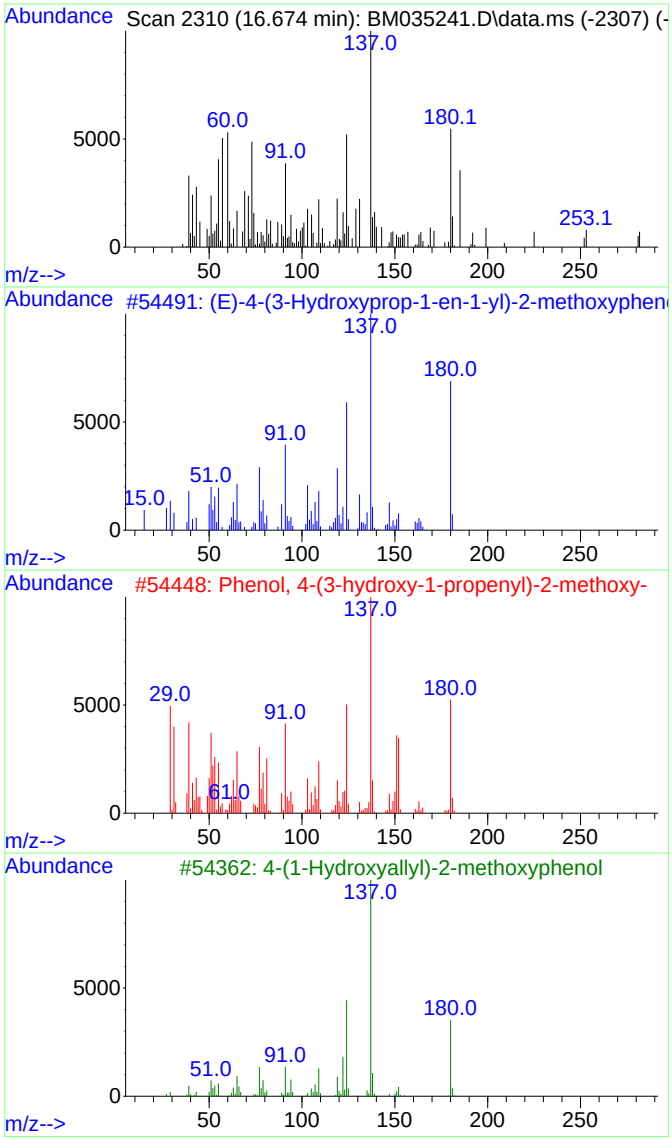
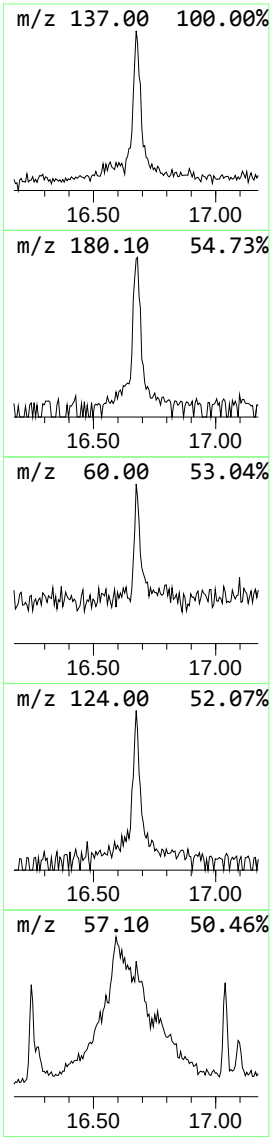
****
Peak Number 1 (E)-4-(3-Hydroxyprop-1-en-1... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.674	2.22 ng	122764	Phenanthrene-d10	17.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-4-(3-Hydroxyprop-1-en-1-yl)-...	180	C10H12O3	032811-40-8	64
2	Phenol, 4-(3-hydroxy-1-propenyl)...	180	C10H12O3	000458-35-5	52
3	4-(1-Hydroxyallyl)-2-methoxyphenol	180	C10H12O3	112465-50-6	49
4	2,5-Dihydroxy-4-isopropyl-2,4,6-...	180	C10H12O3	054755-56-5	38
5	2-Propanone, 1-(4-hydroxy-3-meth...	180	C10H12O3	002503-46-0	30





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Operator : CG/JU
Sample : N2978-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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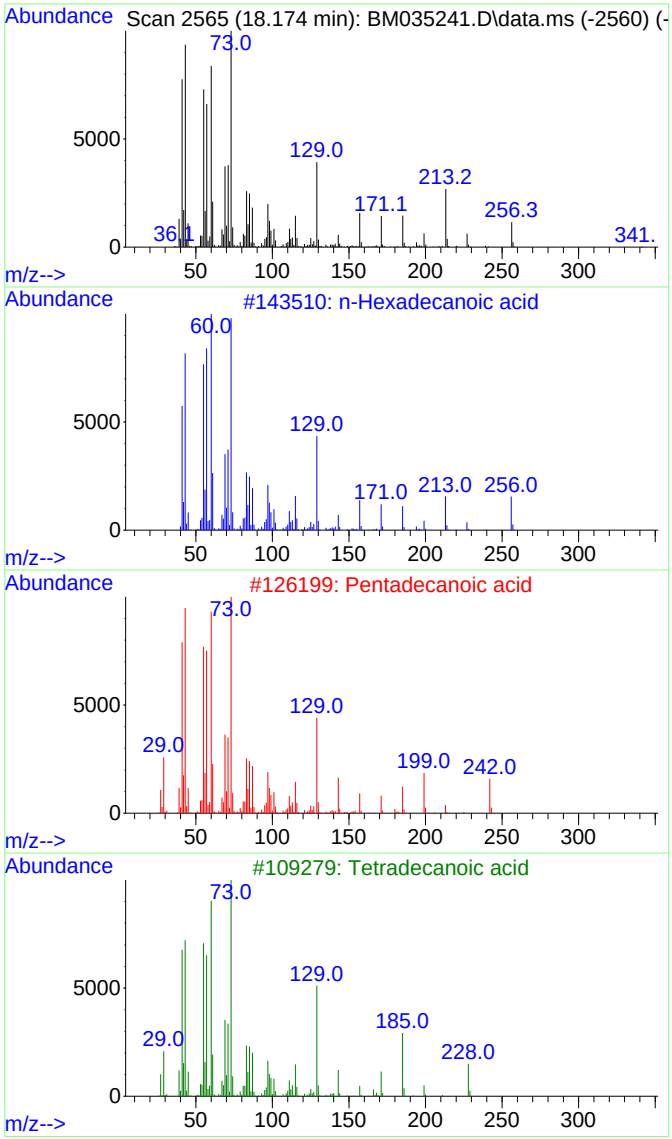
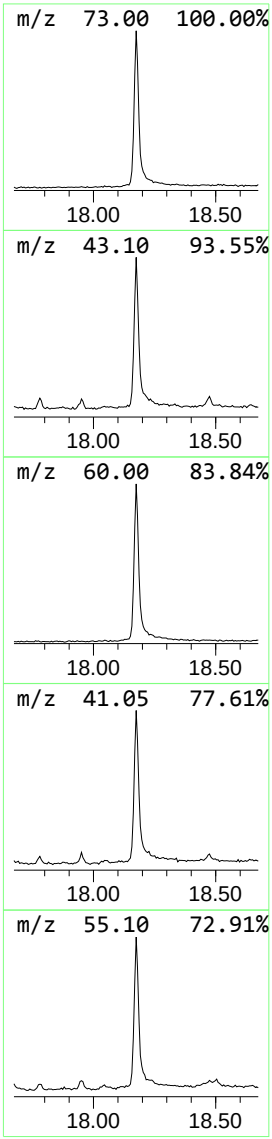
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.174	17.79 ng	984062	Phenanthrene-d10	17.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	62





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Acq On : 25 May 2022 14:03
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Sample : N2978-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-303-20220519

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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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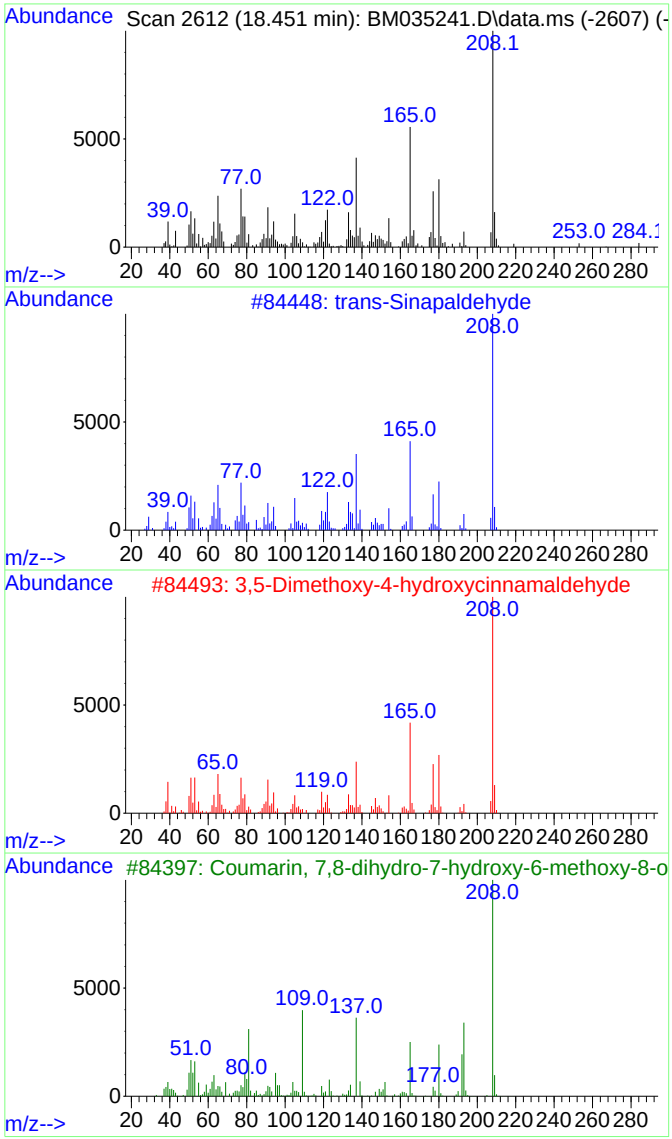
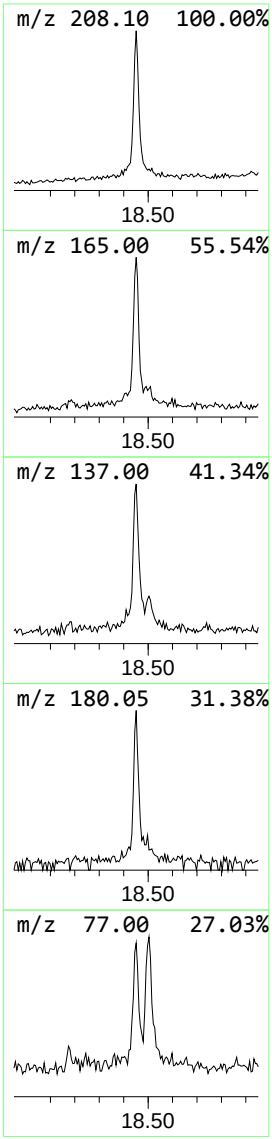
Peak Number 3 trans-Sinapaldehyde Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.451	2.97 ng	164127	Phenanthrene-d10	17.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Sinapaldehyde	208	C11H12O4	004206-58-0	96
2	3,5-Dimethoxy-4-hydroxycinnamald...	208	C11H12O4	087345-53-7	93
3	Coumarin, 7,8-dihydro-7-hydroxy-...	208	C10H8O5	1000263-13-6	58
4	Asarone	208	C12H16O3	002883-98-9	52
5	4-(2-Amino-1,3-thiazol-4-yl)-1,3...	208	C9H8N2O2S	090850-44-5	49





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Data File : BM035241.D
Acq On : 25 May 2022 14:03
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Instrument :
BNA_M
ClientSampleId :
SP-303-20220519

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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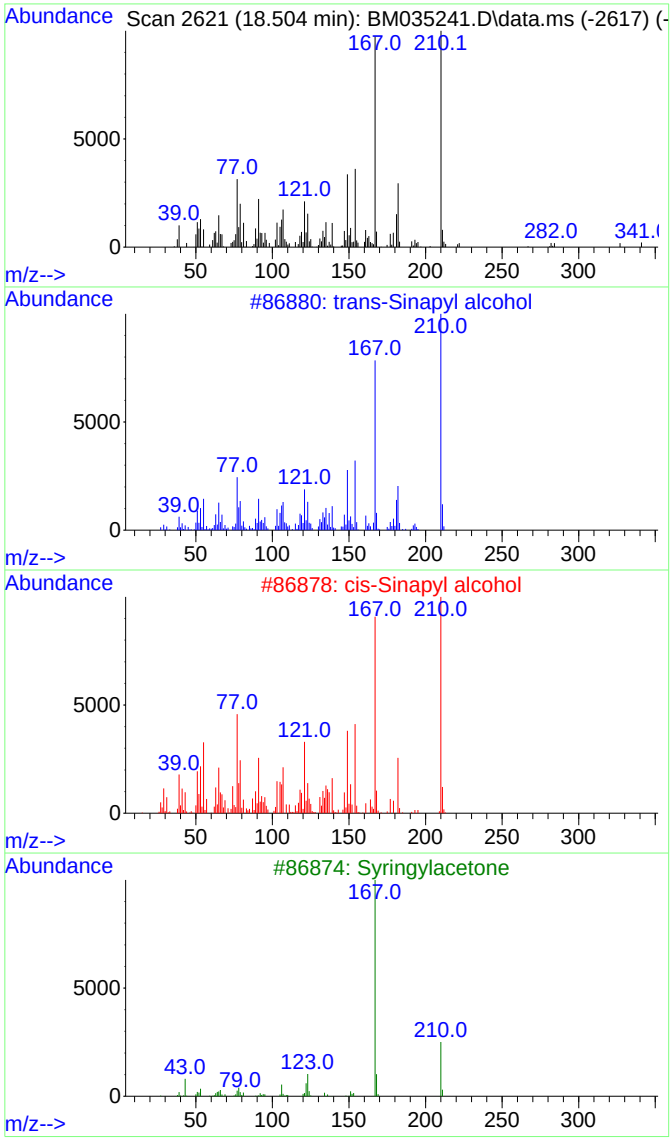
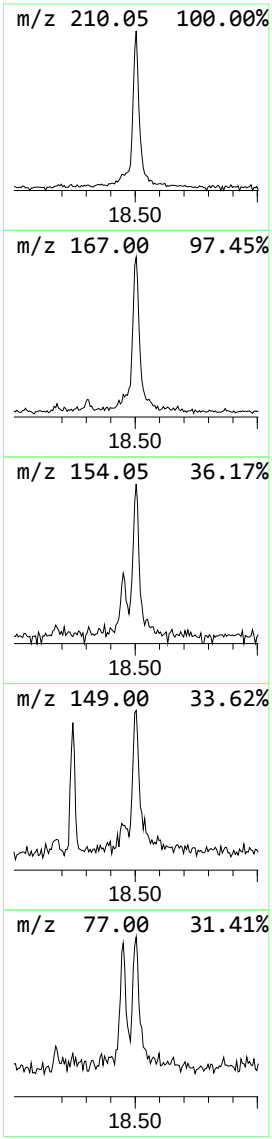
Peak Number 4 trans-Sinapyl alcohol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.504	3.29 ng	181988	Phenanthrene-d10	17.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Sinapyl alcohol	210	C11H14O4	020675-96-1	96
2	cis-Sinapyl alcohol	210	C11H14O4	104330-63-4	49
3	Syringylacetone	210	C11H14O4	019037-58-2	47
4	2H-1-Benzopyran-2-one, 3-chloro-...	210	C10H7ClO3	006174-86-3	30
5	1-Hydroxy-6-methylphenazine	210	C13H10N2O	014031-08-4	30





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ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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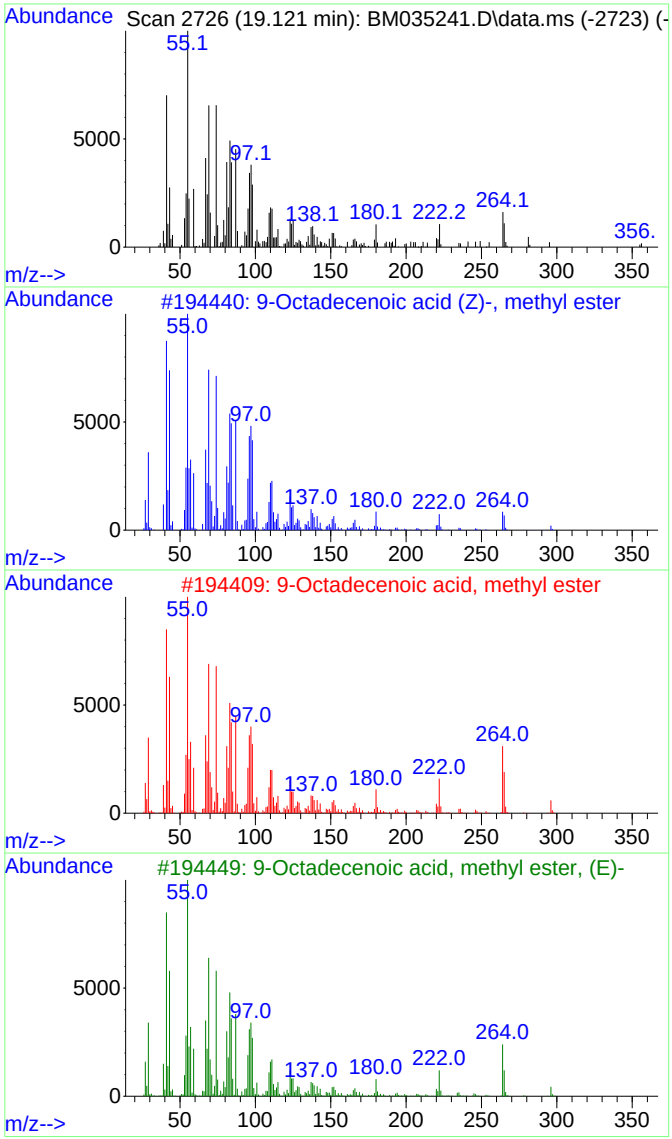
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

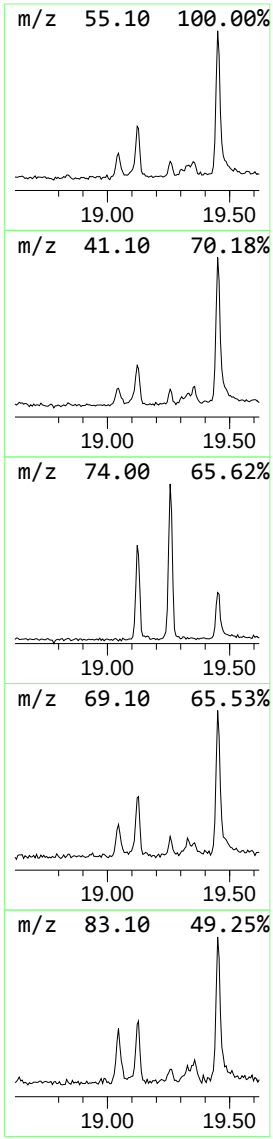
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.121	3.34 ng	184802	Phenanthrene-d10	17.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	94
3	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	94
4	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	94
5	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	91





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TIC Library : C:\Database\NIST20.L
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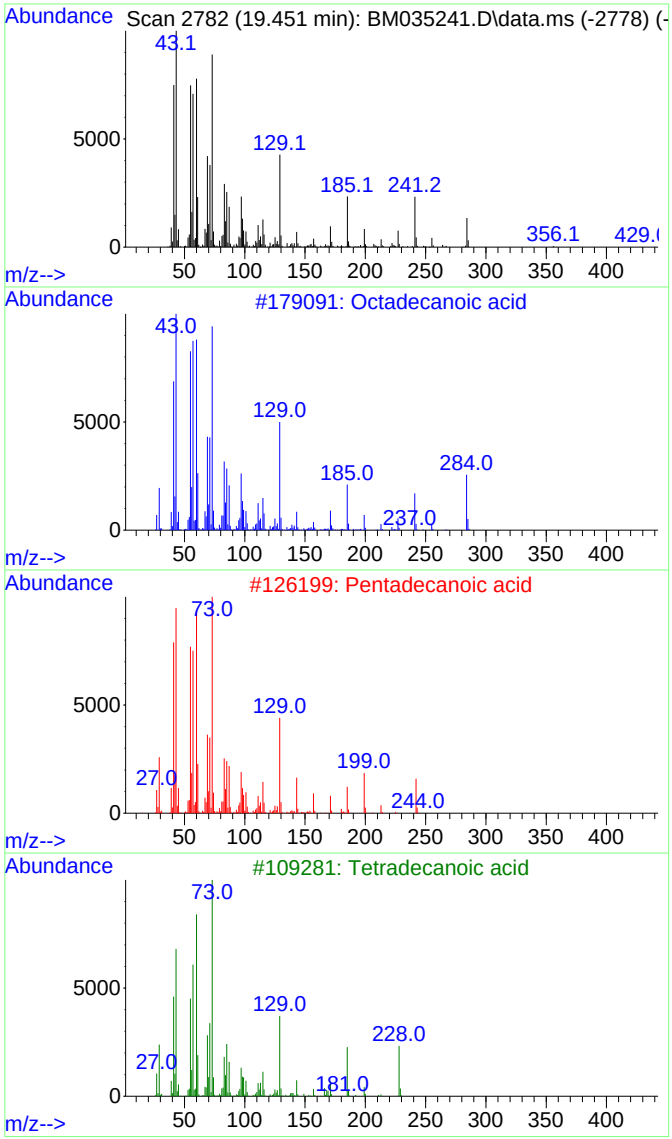
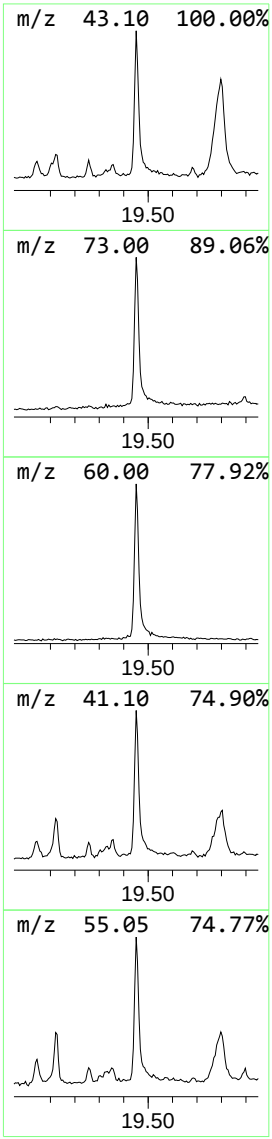
Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.451	9.53 ng	691041	Chrysene-d12	21.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052522\
Data File : BM035241.D
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Sample : N2978-03
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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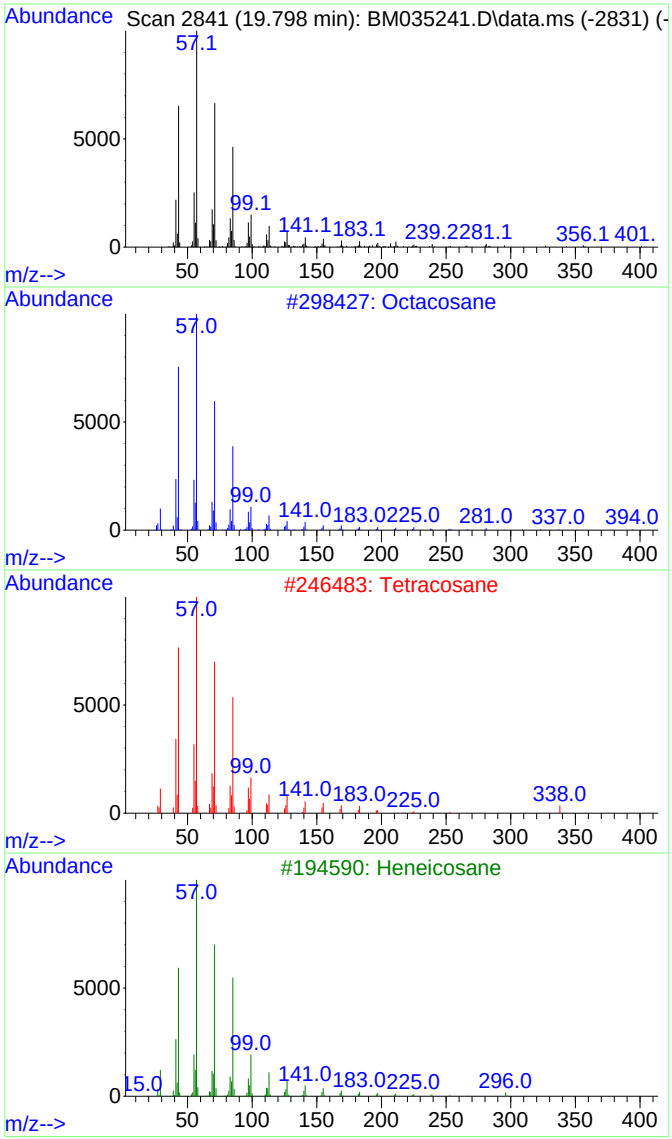
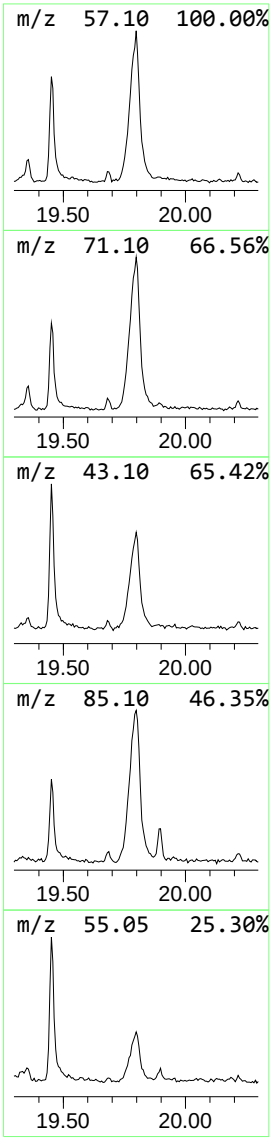
Peak Number 7 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.798	8.63 ng	625927	Chrysene-d12	21.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Triacontane	422	C30H62	000638-68-6	91
5	Tetratetracontane	619	C44H90	007098-22-8	91





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TIC Library : C:\Database\NIST20.L
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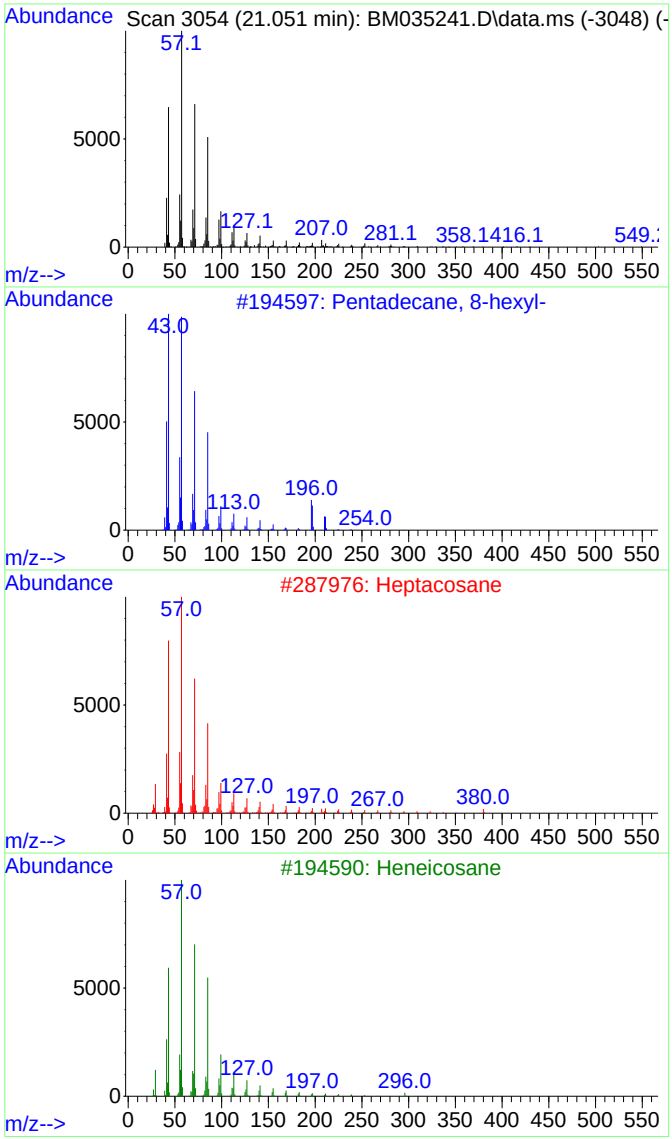
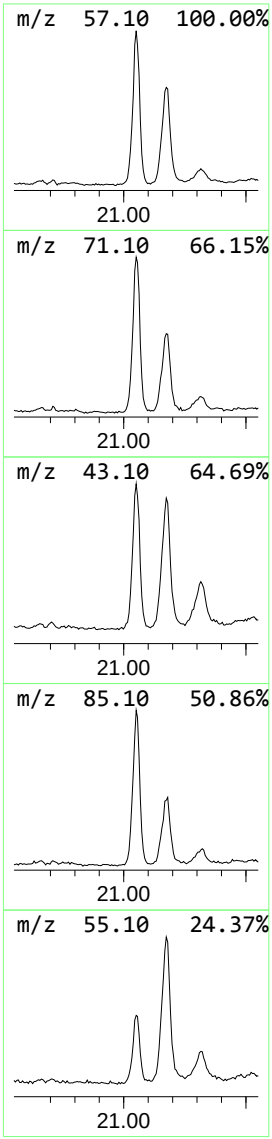
Peak Number 8 Pentadecane, 8-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.051	9.92 ng	719637	Chrysene-d12	21.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	93
2	Heptacosane	380	C27H56	000593-49-7	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
5	Eicosane	282	C20H42	000112-95-8	87





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Acq On : 25 May 2022 14:03
Operator : CG/JU
Sample : N2978-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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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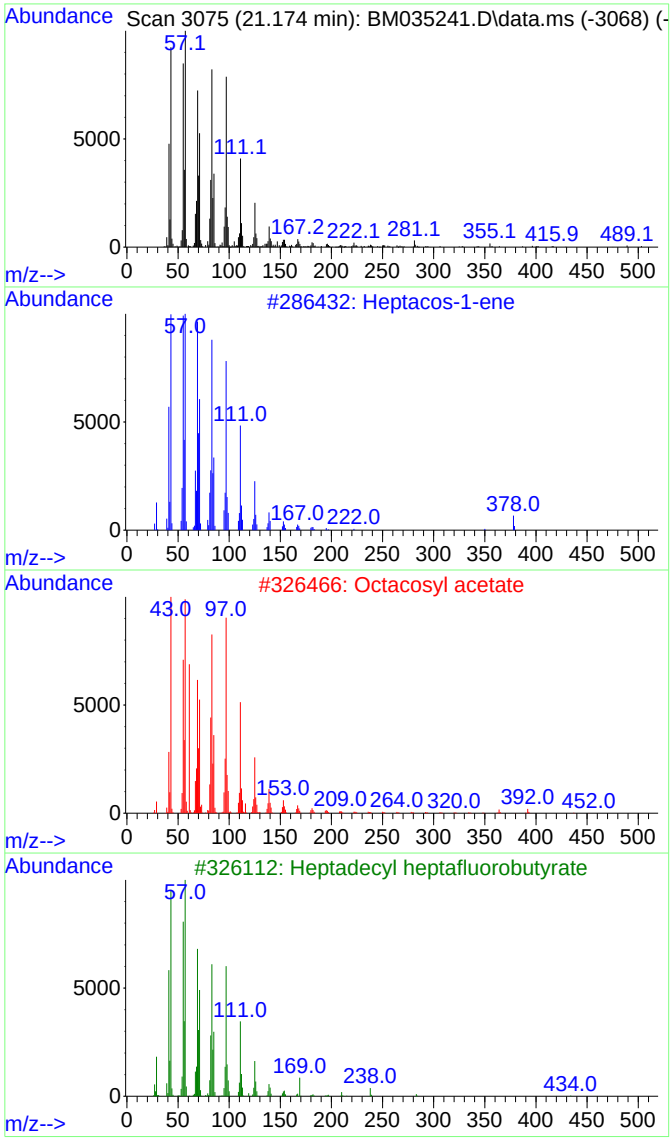
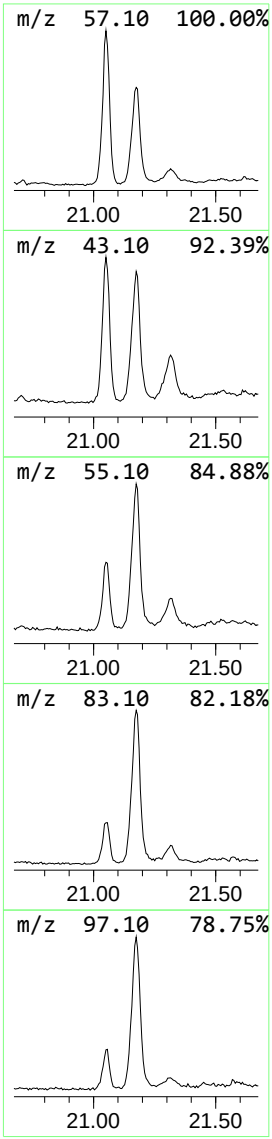
Peak Number 9 Heptacos-1-ene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.174	14.92 ng	1082350	Chrysene-d12	21.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacos-1-ene	378	C27H54	015306-27-1	94
2	Octacosyl acetate	452	C30H60O2	018206-97-8	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	1-Hexacosene	364	C26H52	018835-33-1	94
5	Octacosanol	410	C28H58O	000557-61-9	94





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Data File : BM035241.D
Acq On : 25 May 2022 14:03
Operator : CG/JU
Sample : N2978-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-303-20220519

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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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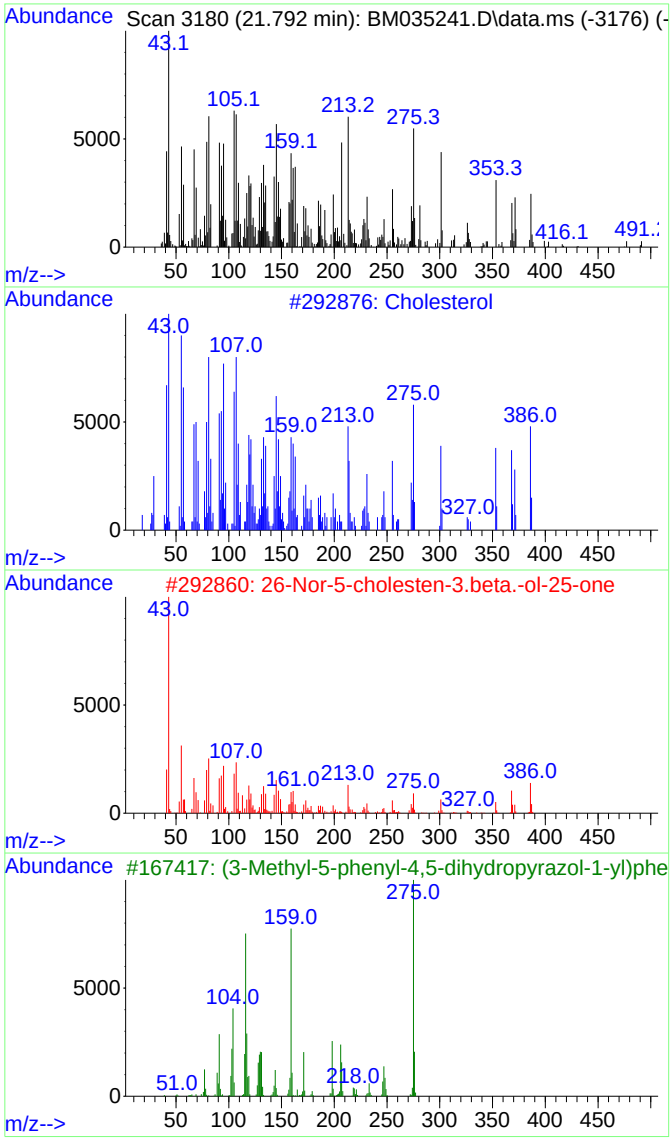
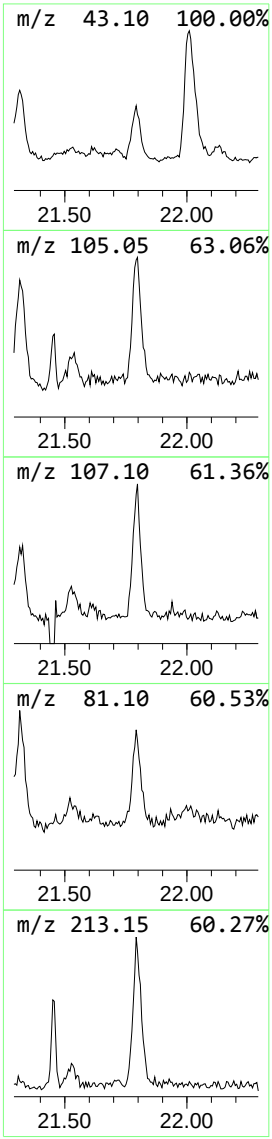
Peak Number 10 Cholesterol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.792	7.04 ng	510682	Chrysene-d12	21.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholesterol	386	C27H46O	000057-88-5	64
2	26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	64
3	(3-Methyl-5-phenyl-4,5-dihydropy...	275	C18H17N3	1000306-61-9	35
4	Cholestane-3,5-diol, 5-acetate, ...	446	C29H50O3	041721-93-1	25
5	4-(4-Isopropyl-trans-6-methyl-3-...	386	C20H26N4O4	1010243-17-3	11





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052522\
Data File : BM035241.D
Acq On : 25 May 2022 14:03
Operator : CG/JU
Sample : N2978-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-303-20220519

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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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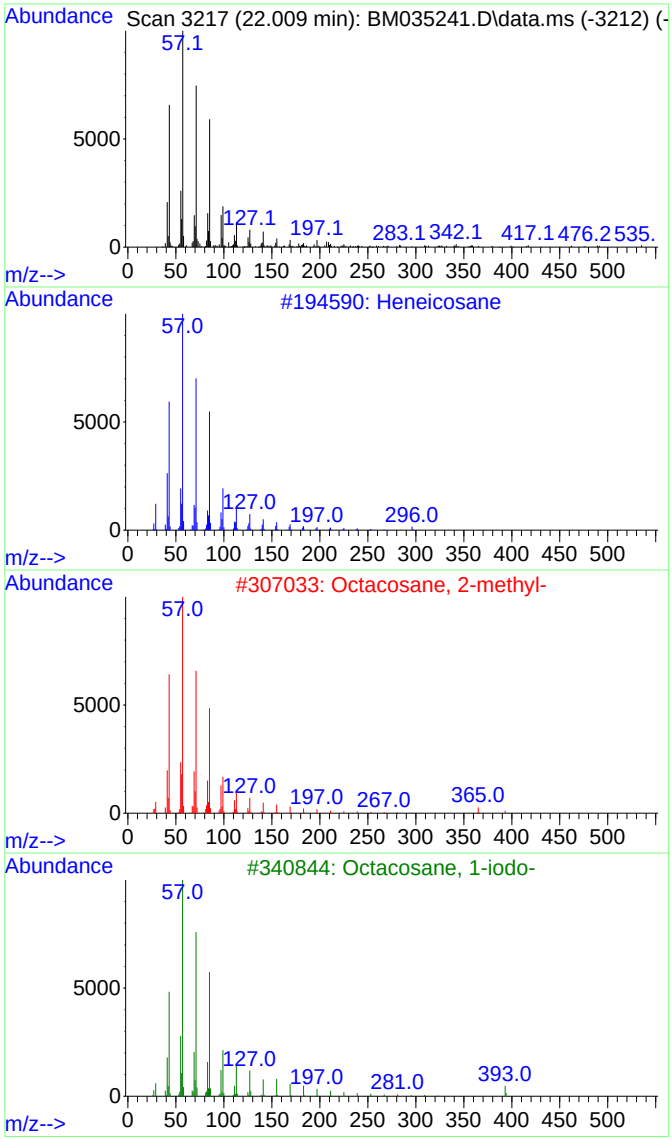
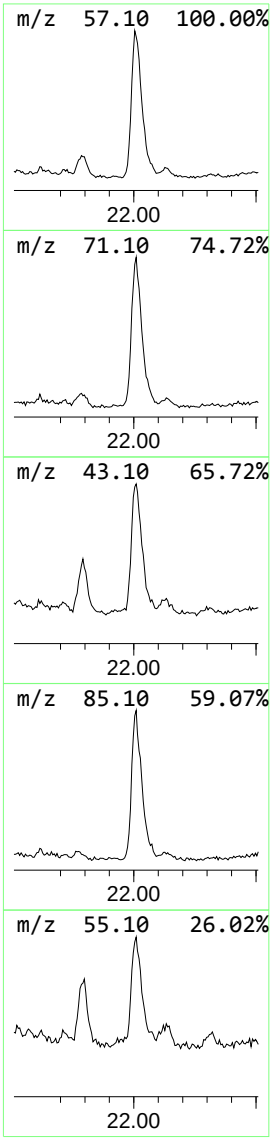
Peak Number 11 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.009	7.02 ng	509261	Chrysene-d12	21.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	96
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3	Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052522\
Data File : BM035241.D
Acq On : 25 May 2022 14:03
Operator : CG/JU
Sample : N2978-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-303-20220519

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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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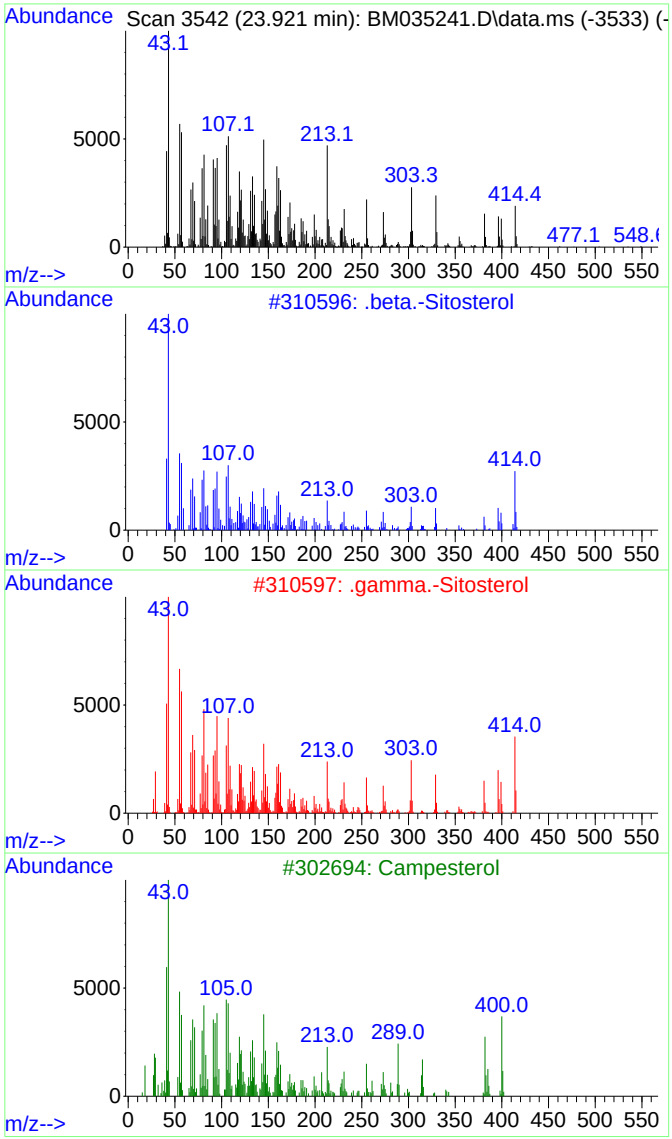
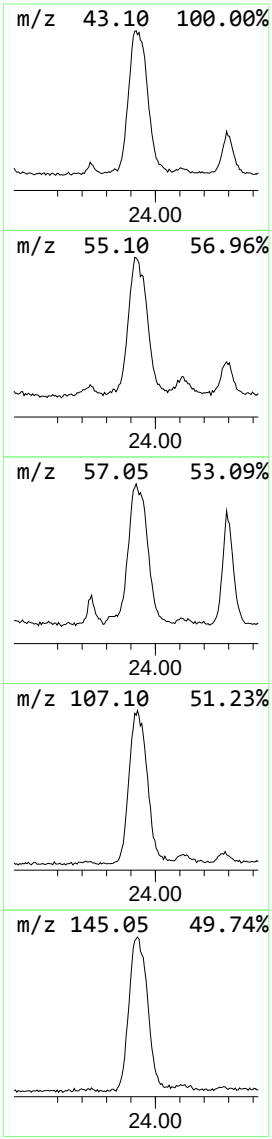
Peak Number 12 .beta.-Sitosterol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.921	75.10 ng	5867900	Perylene-d12	23.833

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol	414	C29H50O	000083-46-5	98
2	.gamma.-Sitosterol	414	C29H50O	000083-47-6	98
3	Campesterol	400	C28H48O	000474-62-4	46
4	(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	45
5	(3S,8S,9S,10R,13R,14S,17R)-17-((...	428	C30H52O	020194-50-7	40





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052522\
Data File : BM035241.D
Acq On : 25 May 2022 14:03
Operator : CG/JU
Sample : N2978-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-303-20220519

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(E)-4-(3-Hydrox...	16.674	2.2	ng	122764	4	17.269	1106490	20.0
n-Hexadecanoic ...	18.174	17.8	ng	984062	4	17.269	1106490	20.0
trans-Sinapalde...	18.451	3.0	ng	164127	4	17.269	1106490	20.0
trans-Sinapyl a...	18.504	3.3	ng	181988	4	17.269	1106490	20.0
9-Octadecenoic ...	19.121	3.3	ng	184802	4	17.269	1106490	20.0
Octadecanoic acid	19.451	9.5	ng	691041	5	21.451	1450680	20.0
Octacosane	19.798	8.6	ng	625927	5	21.451	1450680	20.0
Pentadecane, 8-...	21.051	9.9	ng	719637	5	21.451	1450680	20.0
Heptacos-1-ene	21.174	14.9	ng	1082350	5	21.451	1450680	20.0
Cholesterol	21.792	7.0	ng	510682	5	21.451	1450680	20.0
Heneicosane	22.009	7.0	ng	509261	5	21.451	1450680	20.0
.beta.-Sitosterol	23.921	75.1	ng	5867900	6	23.833	1562690	20.0